DataApex
Clarity™
CHROMATOGRAPHY SOFTWARE

USER GUIDE

Clarity Software ENG

Code/Rev.: M021/100B
Date: 2025-02-05

DataApex Ltd.
Petrzilkova 2583/13
158 00 Prague 5
Czech Republic

Phone: +420 251 013 400
clarity@dataapex.com
www.dataapex.com

Clarity®, DataApex® and ® are trademarks of DataApex Ltd. Microsoft® and Windows™ are trademarks of Microsoft Corporation.
DataApex reserves the right to make changes to manuals without prior notice. Updated manuals can be downloaded from www.dataapex.com.

Author: DR

Contents

1 Installation **1**
1.1 Installing Clarity Software 1
1.2 Updating Clarity Software 6
1.3 Installing Colibrick 13
1.4 Installing a Rockey USB dongle 14
1.5 Connecting a chromatograph analogue output to Clarity 16
1.6 Installing Multicom 17
2 Configuring the Chromatography Station **20**
2.1 Obtaining information about Clarity configuration 20
2.2 Setting the number and type of instruments 21
2.3 Adding a new device 22
2.4 Configuring a device 25
2.5 Setting the options for sending the method to the instrument 27
2.6 Assigning digital input and output to start acquisition 28
2.6.1 Data Inputs & Outputs 29
2.6.1.1 External Start Digital Input 29
2.6.1.2 Ready Digital Output 30
2.6.1.3 Settings Examples 30
2.7 Setting a custom image and a name for an instrument 30
2.8 Tablet mode 31
3 User Accounts **34**
3.1 Creating User Accounts 34
3.2 Managing User's Passwords 34
3.3 Managing User Accounts 34
3.4 Creating a new user account 35
3.5 Restricting access 35
3.6 Duplicating a user account 36
3.7 Sharing user settings among users 37
3.8 Setting a password for the first time 38
3.9 Logging in without a password 39
3.10 Changing a user password 39
3.11 Disabling a user account 41
3.12 Deleting a user account 42
4 Proposed workflow for routine analysis **44**
5 Method Setup **45**
5.1 Setting up a method 45

5.2 Setting up a slow flow rate increase and decrease on your LC pump 50
6 Event Table **54**
6.1 How to make a mark in a chromatogram during acquisition 54
6.2 Signal out of range indication 55
7 Data Acquisition **58**
7.1 Running a single analysis 58
7.2 Pre-evaluating a chromatogram during acquisition 59
7.3 Creating and running a sequence 59
7.4 Editing the template for new sequences 60
7.5 Shut down after finishing a sequence 61
8 Device Monitor **63**
8.1 How to set parameters during run 63
8.2 How to directly control LC gradient pumps during run 64
9 Chromatogram Editing **66**
9.1 How to integrate a chromatogram 66
9.1.1 Setting the integration interval 70
9.1.2 Modifying Global parameters 71
9.1.3 Modifying the beginning and the end of a peak 74
9.1.4 Removing a peak from integration manually 74
9.1.4.1 Baseline - Lock 75
9.1.4.2 Peak - Hide (and Show) 75
9.1.5 Changing the position of a peak separating line 75
9.1.6 Separating rider peaks by tangent 76
9.1.7 Adding a new peak manually 78
9.1.8 Splitting unresolved peaks using Add positive 79
9.2 Saving the chromatogram method as a template method 80
9.3 Adding a peak to a group 81
9.4 Removing a peak from a group 82
9.5 Adding text and lines to a chromatogram 83
9.6 Working with individual signals of a multisignal chromatogram smoothly 85
9.6.1 Individual scaling of signals 85
9.6.2 Graying out 86
9.6.3 Hiding the signals temporarily 87
10 Calibration **90**
10.1 Creating a new calibration 90
10.2 Adding a new calibration level 94
10.3 Creating a model calibration for calibration cloning 95
10.4 Setting a calibration in a chromatogram 97
10.5 Setting a calibration in a method 99

10.6 Adjusting a calibration 100
10.7 Recalibrating a calibration 108
10.8 Recalibrating automatically using a sequence 110
10.9 Calibrating using clone on first recalibration 112
10.10 Calibration - Advanced topics 114
10.10.1 Creating a multisignal calibration 114
10.10.2 Using Internal Standard (ISTD) in calibration 124
10.10.3 Calibrating with manually entered Response Factors 127
10.10.4 Compensating for response drift using bracketing 130
10.10.5 Improving quantification with the standard addition method 135
10.10.5.1 How the concentration is calculated 139
10.10.6 Using a reference peak to improve compound identification 140
10.10.7 Using Calculate By to determine the amount of a compound with no standard available 141
10.10.8 Normalized Area % Calculation 142
10.10.9 Normalized Amount % Calculation 142
10.10.10 How to use Kováts Retention Indexes 145
11 Batch Processing 149
11.1 Reprocessing whole sequence 149
11.2 Reprocessing whole sequence while using calibration cloning 150
11.3 Reprocessing by selected method 151
11.4 Performing Post-run Options from Batch dialog 152
12 Results and Calculations 154
12.1 User Columns 154
12.2 User Variables 156
12.3 Signal to Noise Ratio Calculation 160
12.3.1 Noise Parameter Evaluation 160
12.3.2 Calculating Signal to Noise Ratio 161
12.4 How to calculate Relative Retention Time 162
12.4.1 Relative Retention Time calculation based on an existing peak 162
12.4.2 Relative Retention Time based on the Unretained Peak variable 164
12.5 How to calculate Peak to Valley Ratio 165
12.6 How to handle not-found compounds in your calculations 167
12.7 How to display older results when linked calibration is modified 169
12.8 Calculating percentage content of a compound in a solid sample 171
12.9 Comparing the results from several chromatograms 173
12.10 Confirming the identity of a compound by using the signal ratio 175
13 Data Reports 178
13.1 Setting up a report style for printing 178

13.2 Printing or previewing a report 179
13.3 Creating a report style (example) 183
13.4 Printing the summary table 189
14 File Management 191
14.1 Setting up project directories 191
14.2 Creating a new project 192
14.3 Creating customized file names automatically 193
14.4 Storing chromatograms into subfolders 196
15 Import and Export Data 198
15.1 Importing a chromatogram into Clarity 198
15.2 Exporting a chromatogram from Clarity to a different chromatography data station 199
15.3 Exporting data from Clarity 200
15.4 Exporting data for LIMS 201
15.5 Exporting sequence 206
15.6 Importing sequence 207
15.7 Exporting a chromatogram as a picture 209
16 Mathematical Operations 210
16.1 Extract chromatogram's signal using Mathematical Operations 210
16.2 Subtraction of various chromatograms using Mathematical Operations 210
16.3 Copying of chromatogram using Mathematical Operations 211
17 Archive and Restore 214
17.1 Archiving a project (Creating an Archive) 214
17.2 Restoring a project from an archive 215
17.3 Archiving specific files (Creating an Archive) 216
17.4 Restoring a file from an archive 217
18 Managing the Chromatography Station 219
18.1 Enabling instruments to be used by Clarity2Go application 219
18.2 Locking/Auto Locking a Clarity Instrument 221
18.3 Unlocking a Clarity Instrument 223
18.4 Taking control of Clarity Instrument 223
18.5 Monitoring Events and Operations in Clarity 225
18.6 Controlling Clarity from an external application 227
18.7 Starting a sequence from Clarity at a defined time 227
19 Clarity in specific scenarios 229
19.1 Clarity in the classroom 229
19.1.1 Creating User Accounts 229
19.1.2 Setting the directories 229
19.1.3 Transferring the projects 229

19.1.4 Backing up important files 229
19.1.5 Bonus Tip: Simulated Measurement 230
20 Utilities 231
20.1 Checking that the software has been installed correctly (Installation Qualification - IQ) 231
20.2 Editing Clarity profiles for different analyses using the Launch Manager 232
20.3 Creating a duplicate configuration using the Launch Manager 234
21 Best Practices for Using Clarity Effectively 239
21.1 Respect Clarity's file structure 240
21.2 Avoid switching Windows OS users and entering Sleep mode 242
21.3 Protect Clarity from unexpected shutdowns 243
22 Troubleshooting 244
22.1 Missing HW key 245
22.2 Failed to open file for writing 245
22.3 The User Code is not accepted 246
22.3.1 The User Code is not valid for version x.y 246
22.3.2 Wrong User Code 246
22.3.3 Wrong Software Version 247
22.4 Trial Expired 247
22.5 The XX file is corrupted or missing 248
22.5.1 Clarity.psw file 248
22.5.2 Configuration *.cfg file 249
22.5.3 Project *.prj file 249
22.6 Data Acquisition - Disabled 250
22.7 Data Acquisition - Simulated 251
22.8 Clarity is unable to find HW key 253
22.9 How to create a dump (*.dmp) file from running Clarity 253

To facilitate the orientation in the **User Guide** manual and **Clarity** chromatography station, different fonts are used throughout the manual. Meanings of these fonts are:

Open File (italics) describes the commands and names of fields in **Clarity**, parameters that can be entered into them or a window or dialog name.
WORK1 (capitals) indicates the name of the file and/or directory.
ACTIVE (capital italics) marks the state of the station or its part.
Chromatogram (blue underlined) marks clickable links referring to related chapters.

The bold text is sometimes also used for important parts of the text and the name of the **Clarity** station. Moreover, some sections are written in format other than normal text. These sections are formatted as follows:

Note: Notifies the reader of relevant information.

Caution: Warns the user of possibly dangerous or very important information.

Marks the problem statement or trouble question.

Description: Presents more detailed information on the problem, describes its causes, etc.

Solution: Marks the response to the question, presents a procedure how to remove it.

1 Installation

Topics covering installation of **Clarity** software, **Colibrick**, **Multicom**, etc. Also the connection between **Clarity** and chromatograph is explained.

1.1 Installing Clarity Software

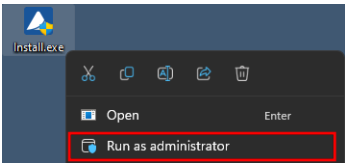
These are the basic steps you have to follow for the First installation of Clarity.

First installation of the software (since version 9.0)

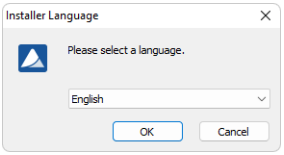
1. Install the software BEFORE connecting any hardware.

   More Info:

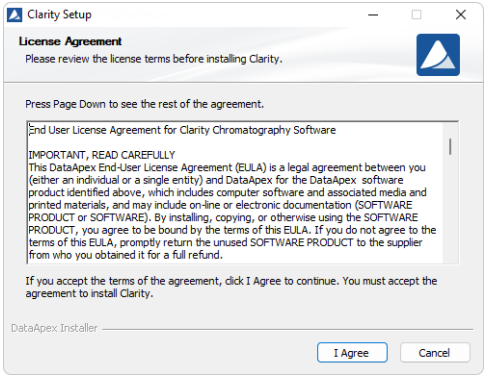
   - The software can be installed by inserting the installation USB and running install.exe or by downloading the installation from the Downloads at our website.
   - On administered systems use „*Run as Administrator*“ from intended User account. Administered systems are managed by an administrator and users using the PC may not have administrator privileges. Insufficient privileges may result in:
     - Clarity not being installed.
     - When installed from Administrator account, the installation directory may be read only for users with limited privileges and the station will be inoperable.



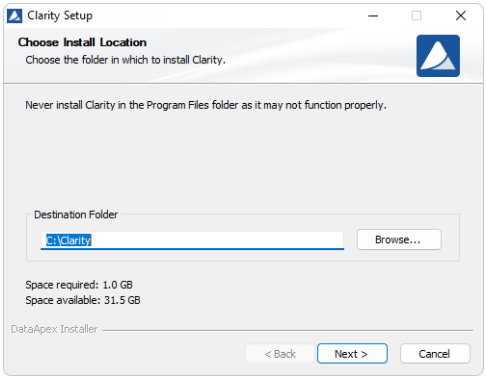
2. Select the language.



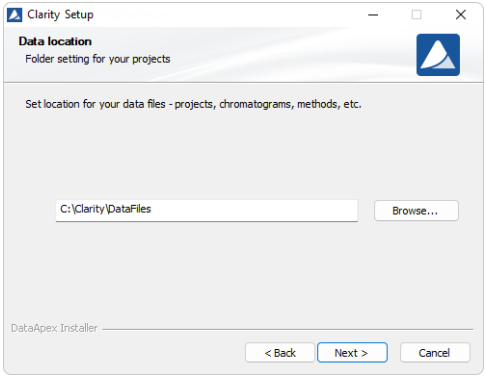
3. Confirm the License Agreement. It is possible to continue only in case you agree with the statement.



4. Choose the destination folder. The user must have Read/Write/Modify access to the installation directory.

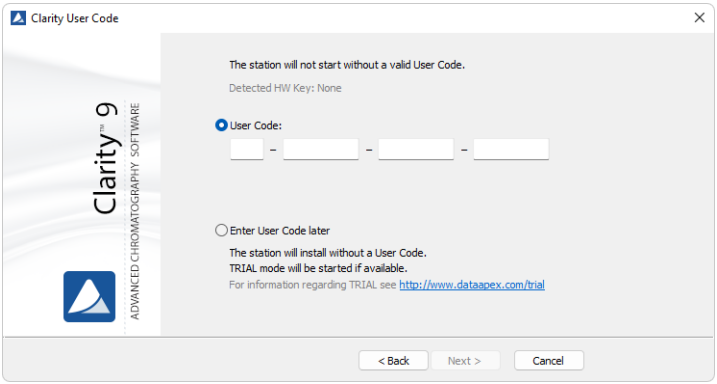


5. Set location for your data files. C:\CLARITY\DataFiles is set by default. Notice that Data location folder name cannot contain following characters / : * ? " < > | and also cannot start or end with a space and cannot end with a dot.



6. Enter the User code corresponding to your hardware key or select *Enter User Code later* to start 30-day Trial.

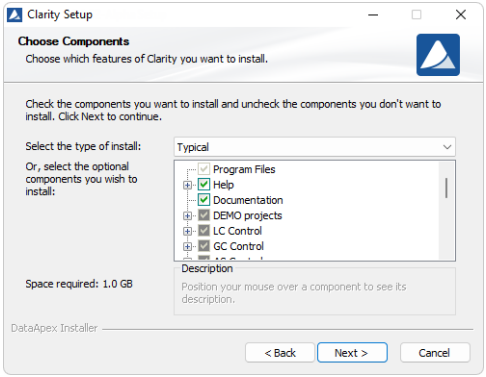
Note: The user code can be found on the back side of the card provided with the Installation USB. Alternatively, you can contact DataApex support to obtain one.



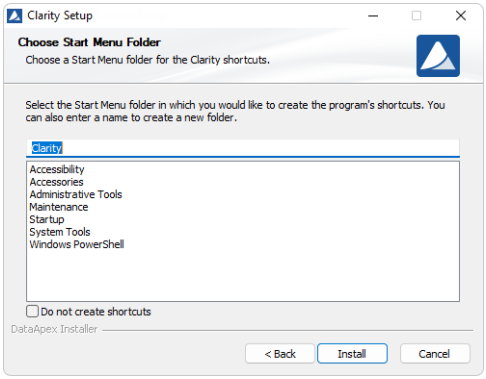
7. Select the type of installation. Make sure that control module for your device is selected to be installed.

Note: In most cases "Typical" should be selected. "Custom"/"Full" installation is necessary e.g., for Agilent and other devices controlled via ICF, DANI devices and few others.

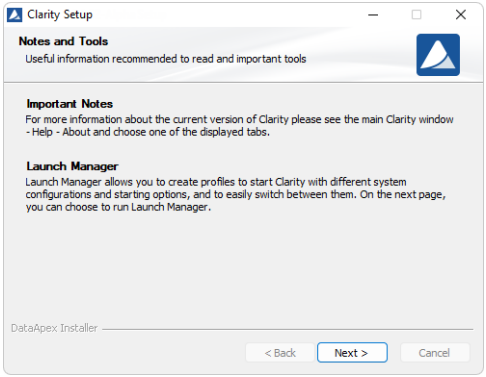
Note: List only contains names of original devices. If you can't find your device, even though it is stated as controlled, it is most likely an OEM version of different device.



8. Select the Start Menu folder for the shortcut or create a new one. After clicking *Install* installation process will start.



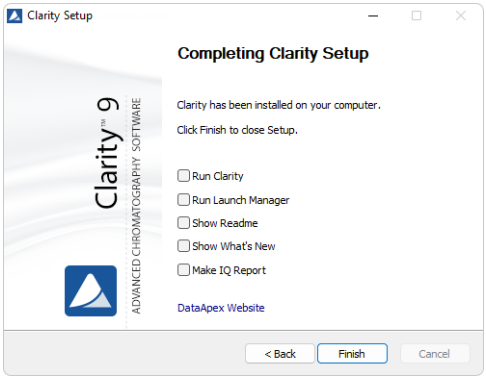
9. Wait for installation to finish. In the end you might be prompted to confirm installation of several hardware drivers.
10. When installation is finished *Notes and Tools window* will be opened.



11. Finally the last window will offer you several actions which may be executed after the installation is completed.

More Info:

- The *Launch Manager* allows you to start Clarity using different profiles that correspond to different configurations and combinations of instruments, projects, methods, etc. For example, different users or groups of users can have the chromatography station configured on the same computer.
- The *Installation Qualification - IQ* (Make IQ report option) is a procedure that confirms that the software has been installed successfully and that the files are in the correct version.



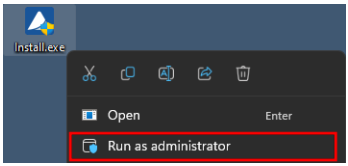
1.2 Updating Clarity Software

These are the basic steps you have to follow to update Clarity.

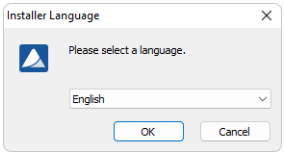
1. Check for the updates: click *Help - Check for Updates...* or download new version of the software from the Downloads at our website.
2. Run the installer.

More Info:

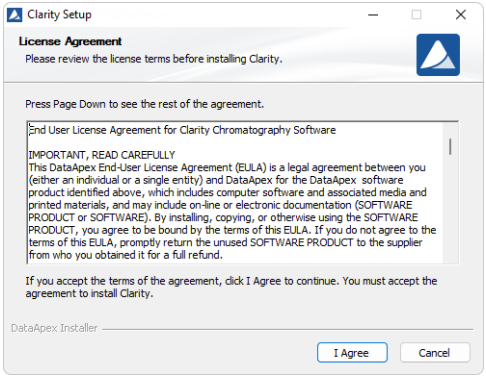
- On administered systems use „*Run as Administrator*" from intended User account. Administered systems are managed by an administrator and users using the PC may not have administrator privileges. Insufficient privileges may result in:
  - Clarity not being installed.
  - When installed from Administrator account, the installation directory may be read only for users with limited privileges and the station will be inoperable.



3. Select the language.



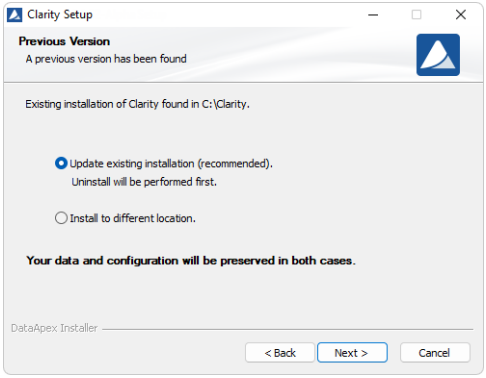
4. Confirm the License Agreement. It is possible to continue only in case you agree with the statement.



5. Previous version of Clarity will be detected. Decide whether to update or preserve this version.

Note: In both cases your data and configuration will be preserved.

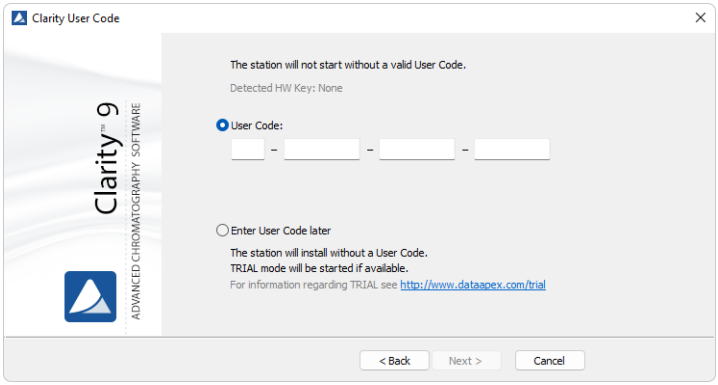
Note: Selecting *Install to different location* will result in presence of two different Clarity version at once (current version will be left as it is and new version will be installed elsewhere).



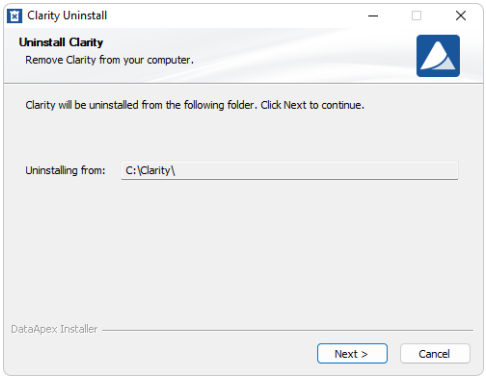
6. If you select to *Update existing installation* it is necessary to confirm the User code (code from current version will be pre-filled).

Caution: Each major version (change of the first version number) since version 9.0 requires new User Code. Make sure that you have a valid User Code for newly installed version before proceeding further. For more information see https://www.dataapex.com/upgrade.

Caution: Downgrading is not supported and might be problematic in some cases.

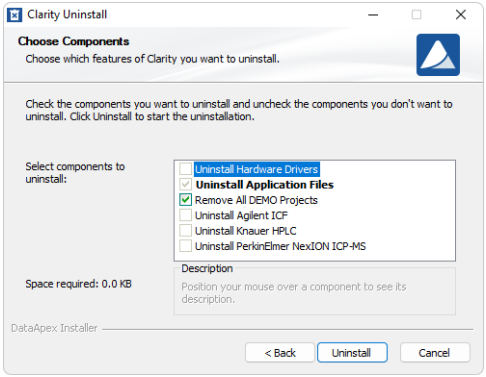


7. Clarity will proceed with uninstallation, following window appears.

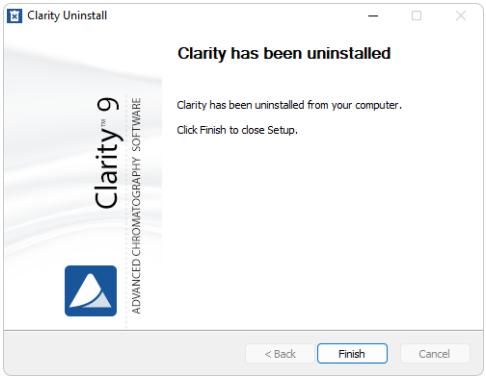


8. Continue to *Choose Components* step and click *Uninstall*.

Caution: When *Remove All DEMO Projects* is selected all files within them will be lost, including any data you saved into their folders. DEMO projects should never be used to store your data.

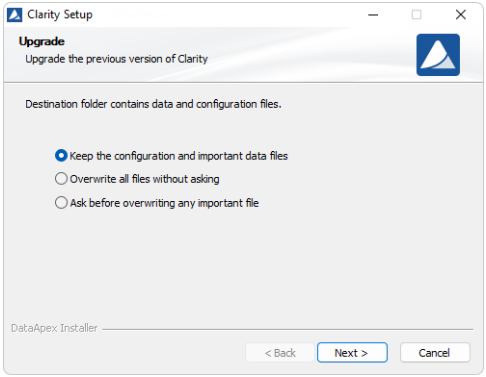


9. Wait for uninstall to finish and click *Finish* in the following window.

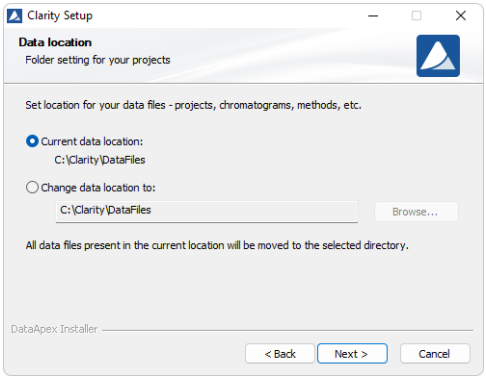


10. Choose what to do with existing data and configuration files.

Caution: It is recommended to select *Keep the configuration and important data files* to preserve all of your settings and data. Other two options might lead to losing important files and should be only used under special circumstances.



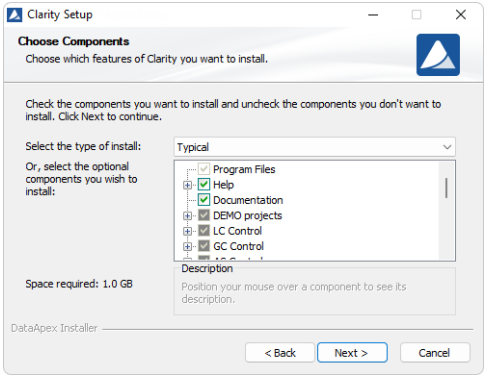
11. Set destination folder for your data files. If data location is changed all data from current version will be moved accordingly.



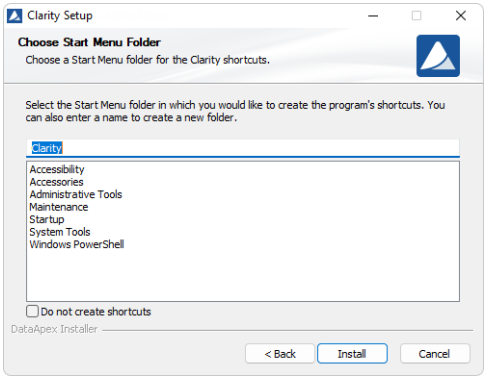
12. Select type of installation. Installation type which was used for current version will be preselected. Make sure that control module for your device is selected to be installed

Note: In most cases "Typical" should be selected. "Custom"/"Full" installation is necessary e.g., for Agilent and other devices controlled via ICF, DANI devices and few others.

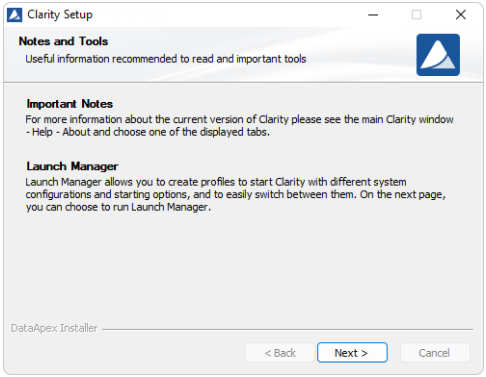
Note: List only contains names of original devices. If you can't find your device, even though it is stated as controlled, it is most likely an OEM version of different device.



13. Select the Start Menu folder for the shortcut or create a new one. After clicking *Install* installation process will start.



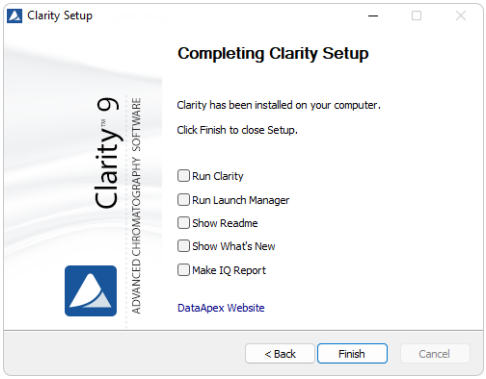
14. Wait for installation to finish.
15. When installation is finished *Notes and Tools window* will be opened.



16. Finally the last window will offer you several actions which may be executed after the installation is completed.

More Info:

- The *Launch Manager* allows you to start Clarity using different profiles that correspond to different configurations and combinations of instruments, projects, methods, etc. For example, different users or groups of users can have the chromatography station configured on the same computer.
- The *Installation Qualification - IQ* (Make IQ report option) is a procedure that confirms that the software has been installed successfully and that the files are in the correct version.



Caution: When upgrading from Clarity 6.2 or older to Clarity 7.0 or newer be aware that there is change in the installation structure - the content of the original installation folder is separated to three new subfolders BIN, CFG and DataFiles. The respective files are moved automatically during update to the new locations if you selected *Update existing installation*. In the rare cases this fails, some files may need to be moved manually.

1.3 Installing Colibrick

Colibrick is an external 24-bit A/D converter designed for acquisition of data from any chromatograph. It uses the USB communication channel and it is powered from the PC.

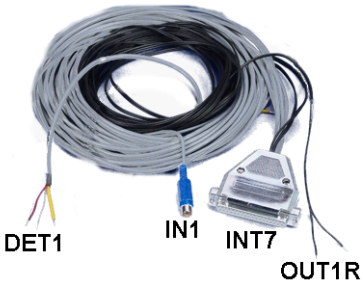
1. First install Clarity.

   More Info:

   - The driver is by default installed in *Typical* installation of Clarity. It can be found in *Hardware* section of *Choose Components* step.
   - The *Colibrick* device is identified by its S/N. If you exchange it by another one later, it will be also necessary to reconfigure it in the *Clarity - System Configuration* dialog.

2. Connect *Colibrick* to a USB port in your computer. It will be detected automatically.

3. Connect the CANNON SUB D 27-pin connector on the (INT7) cable to *Colibrick* back panel.



4. Connect the cables (Starting, Digital output and Analog Signal) to the chromatograph as explained in *Connecting a chromatograph analogue output to Clarity*.
5. Start Clarity and then add the *Colibrick* channels to specific Clarity instruments as explained in *Adding a new device*.
6. Check the LED's on the front panel to find out about the status of *Colibrick* and whether it has been installed properly.

More Info:

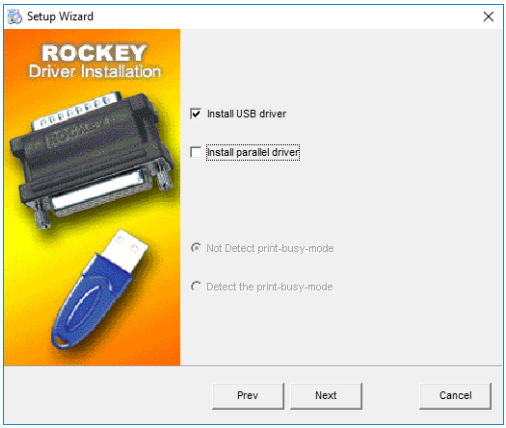
- Ready (orange) LED status Indicates correct installation.
- Data (blue) LED status Indicates connection to the chromatography data station.
- Digital Input (green) LEDs status
  - LED ON - the input status is High (logical "1") or not connected.
  - LED OFF - the input status is Low (logical "0") or connected to the ground (GND).
- Digital Output (red) LEDs status
  - LED ON - the output status is High (logical "1"), the relay contact is opened.
  - LED OFF - the output status is Low (logical "0"), the relay contact is closed.

1.4 Installing a Rockey USB dongle

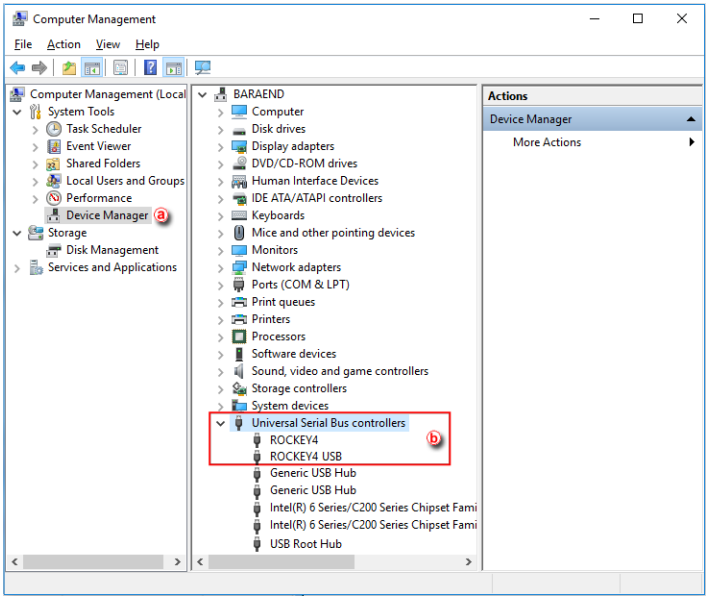
Currently supplied RkNDUSB HW keys use the HID (Human interface device) technology and do not require any drivers.

For old RkUSB keys the drivers will be installed automatically during the installation of Clarity. For this reason it is important to install Clarity before plugging the key. If the installation did not proceed as expected or you may have an old version of Windows, follow the procedure below.

1. First install Clarity.
2. Connect the USB dongle to a USB port on the computer.
3. Install the Rockey drivers by running INSTDRV.EXE in C:\CLARITY\BIN\HW_DRIVERS\ROCKEY\. The following window will appear.
4. Select the Install USB driver option and click on Next to finish the installation.



5. Verify that the driver has been installed correctly. Meaning that the *Device Manager* ⓐ has the item "*Universal Serial Bus Controllers*" - "*Rockey4 USB*" ⓑ .



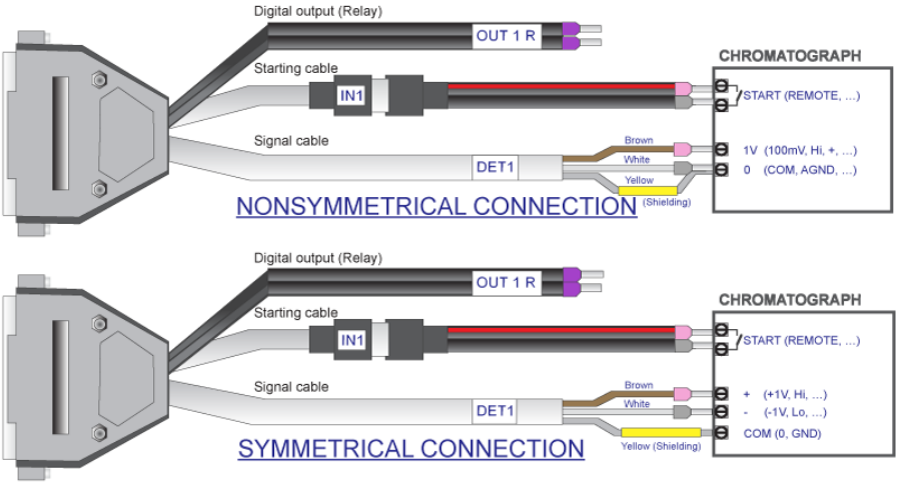
If this does not work, try the following procedure after the installation of Clarity: After connecting the dongle, Windows will detect a new Plug and Play device and the *Found New Hardware Wizard* will appear.

1. Select "*Search for a suitable driver for my device.*"
2. Select "*Specify a location*" and then select the C:\CLARITY \BIN\HW_ DRIVERS\ROCKEY\folder. The rest of the installation will be carried out automatically.

Note: On Windows 10 and Windows 11, the driver for older HW keys (Rockey4USB.sys) can only be installed if Memory Integrity/Core isolation function of Windows Security is turned off. This function is turned on by default. If an incompatible driver is already installed on the computer, it cannot be turned on. But if it is enabled, the driver installation fails with Error code 39.

1.5 Connecting a chromatograph analogue output to Clarity

The Clarity Station cable (INT7) connects the station to the chromatograph and it is a set of Starting, Digital output and Analog Signal cables connected to a CANNON SUB D 27-pin connector.



1. Install your external A/D converter like *Colibrick* (refer to ***Installing Colibrick***) or an A/D converter card (refer to the specific HW manual).
2. Switch off your chromatograph.
3. Connect the bare wires to the chromatograph depending on your equipment, configuration and the following guidelines.

More Info:

- The **Signal cables** "DET 1" to "DET 4" carry the main signal from the chromatograph to the computer. The connection can be asymmetrical or symmetrical.
- The **Starting cables** "IN1" to "IN4" come in pairs, one part connected to the 27-pin connector and ending on a female RCA connector and the other with a male RCA connector and free leads for connection to a starting contact or a button for a manual start.
- The **Digital Output cables** "OUT 1R" to "OUT 4R" end on free leads and they can be used for synchronizing autosamplers.

Caution: The shielding must be connected. It works not only as the shielding, but also as the analogue ground against which measurement takes place. In the case of asymmetrical output of a detector (only two leads/terminals/pins/screws) the shielding must be connected to the white lead! No lead of the signal cable may remain unconnected.

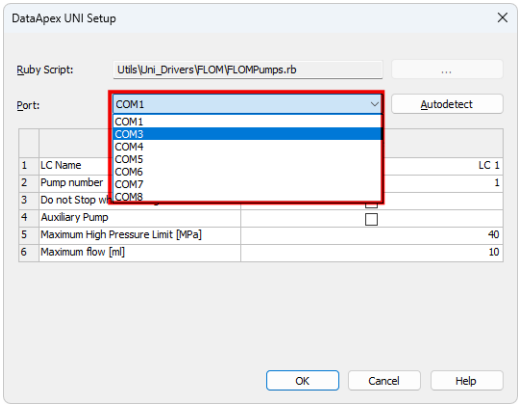
4. Connect the CANNON SUB D 27-pin connector to the A/D convertor.
5. Switch on your computer and your chromatograph.

1.6 Installing Multicom

MultiCOM is a USB to RS232 converter developed for controlling via the RS232 serial interface. It is connected to the PC via the USB port and has 6 serial 9-pin ports. It also has a free USB port for the connection of the ***USB hardware key***.

1. First install Clarity. *Multicom* driver is by default installed in *Typical* installation of Clarity. It can be found in *Utils* section of *Choose Components* step.
2. Connect *Multicom* to a USB port in your computer. It will be detected automatically. LED diodes will be turned on one by one.
3. Connect your devices to the *Multicom* RS232 ports.
4. Start Clarity and then add each device to a specific Clarity instrument as explained in ***Adding a new device***.
5. Select the appropriate port from the list during the device setup.

Note: When using functions like *Autodetect* and *Check* LED diode of selected port will blink. This can be used to find the desired port number on *Multicom*.



6. Check the LEDs on the top panel to find out about the status of *Multicom* and whether it has been installed properly.

More Info:

Green LED status:

- OFF – not connected to USB, the driver is not installed or *Multicom* is in suspend mode.
- ON (Constant) – idle state, no communication.
- BLINKING:
  - Two short consecutive blinks – only sending data from USB to the COM port.
  - Turned off twice consecutively – only receiving data from the COM port into USB.
  - Constant blinking – both sides are receiving and sending data.

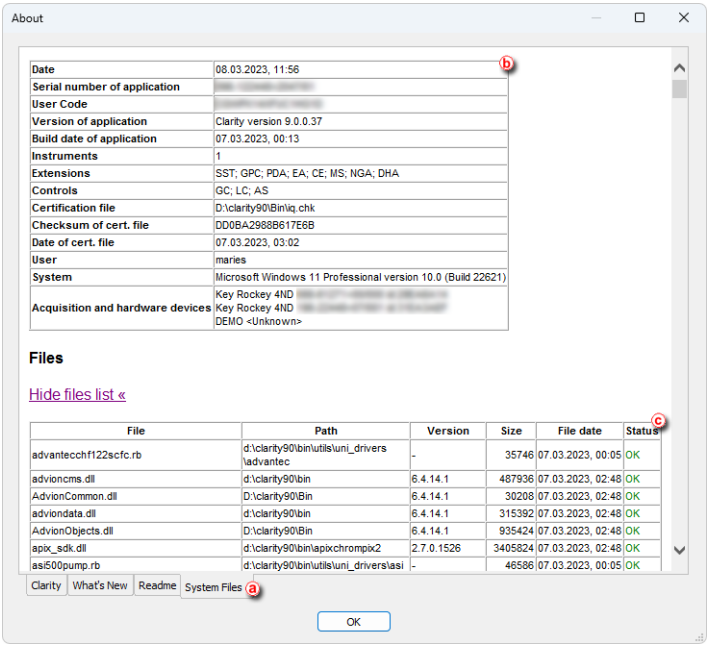
2 Configuring the Chromatography Station

Chapters covering settings in the *System Configuration* dialog.

2.1 Obtaining information about Clarity configuration

To find out information on the supported control modules and Extensions, used A/D converters and purchased Instrument licenses follow this procedure:

1. Open the *About* box: Select *Help - About…* on the *Main* window.
2. Switch to the *System Files* tab ⓐ . Note that it may take a while for Clarity to generate the report.
3. In the first table ⓑ there is info about:
   - Clarity SW version
   - Number of purchased instrument licenses
   - Extensions available
   - The allowed control modules
   - Acquisition and hardware devices
4. Go to the files table ⓒ to find information about the drivers and its status.
   If the status is other than *OK* there may be an issue with the driver. The version of the drivers developed by DataApex should be the same as that of Clarity.



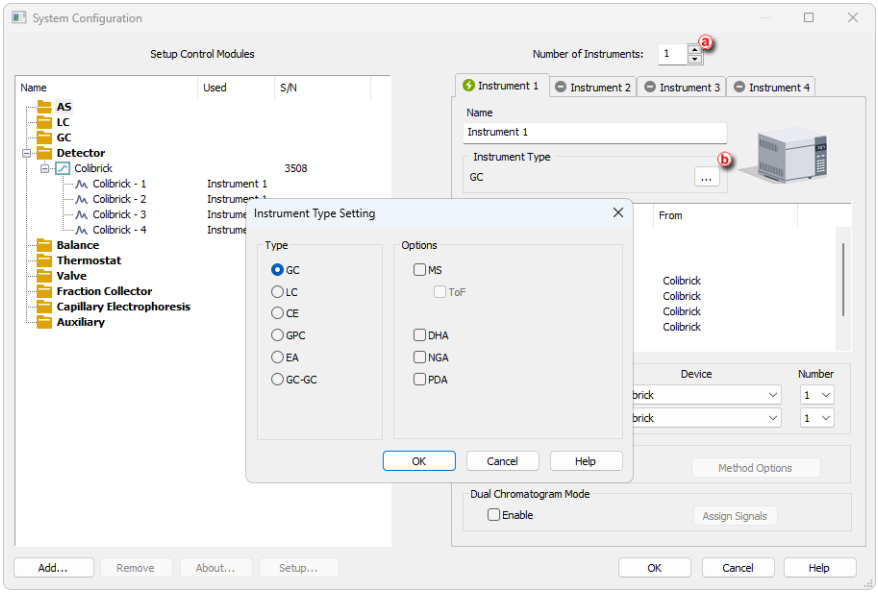
2.2 Setting the number and type of instruments

1. Enter the *System Configuration* dialog: select *System - Configuration…* in the *Main* window.
2. In the *Number of Instruments* field ⓐ you can set a number of instruments, based on bought licenses or you can use non-bought Instrument as the Offline ones.

Note: The Offline instruments can be used for method or sequence preparation, or evaluation of previously measured chromatograms.

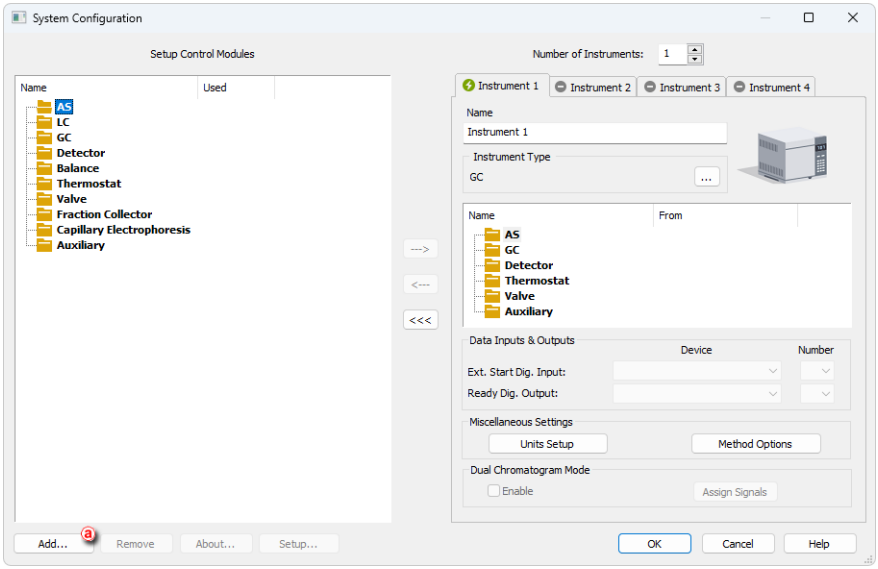
3. Set the *Instrument Type* field ⓑ according to the type of instrument you are using e.g., GC or LC. To be able to assign some of the devices to the *Instrument*, correct *Instrument Type* has to be selected.

Note: To use specific Extension Instrument Types such as GPC, PDA, EA, NGA, etc., you need to have the particular extension license purchased.



2.3 Adding a new device

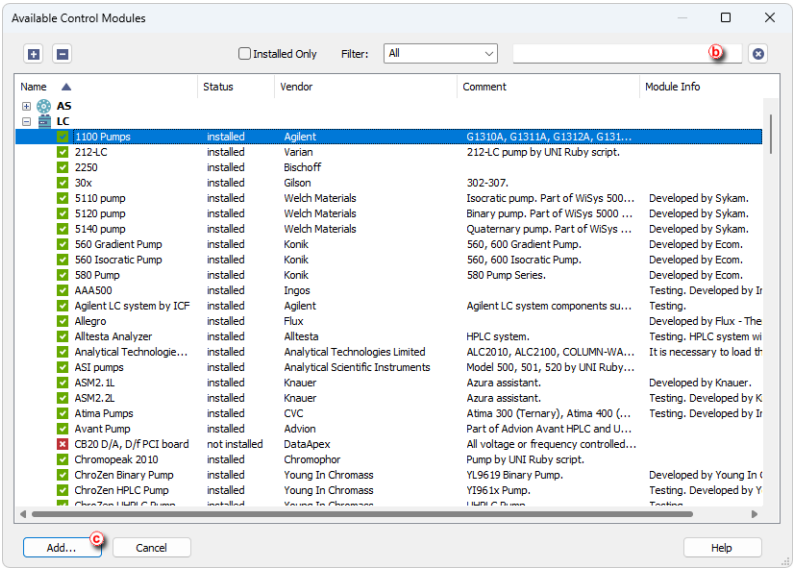
1. Enter the *System Configuration* dialog: select *System - Configuration…* on the *Main* window.



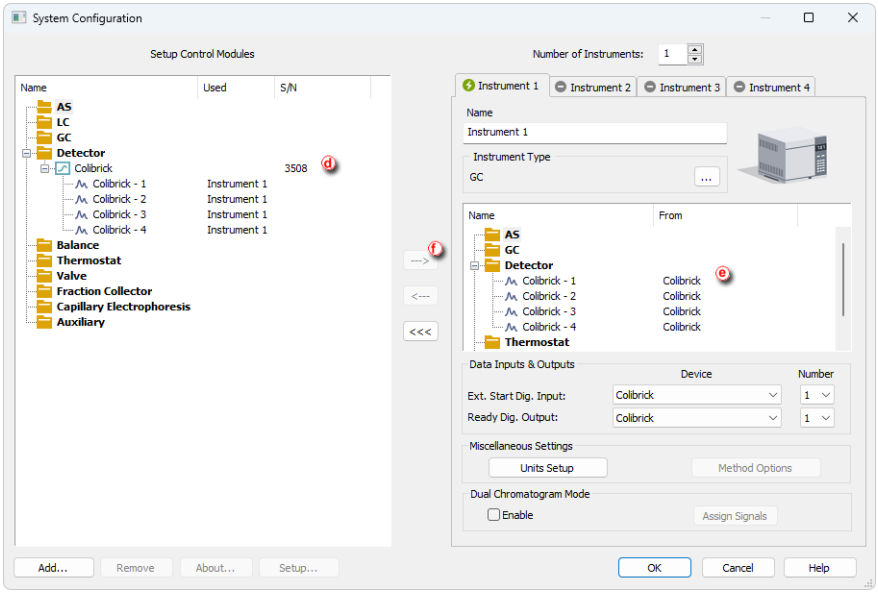
2. If the device you want to add is not in the list, click on *Add* ⓐ and the *Available Control Modules* dialog will open. Here, you can filter the list by typing some text in the filter field ⓑ .

   Note: If the status of the module is *not installed*, double-click the line with this device to see why the module is not installed and how to remedy the situation.

3. Select the device and click on *Add* ⓒ or double-click the line.



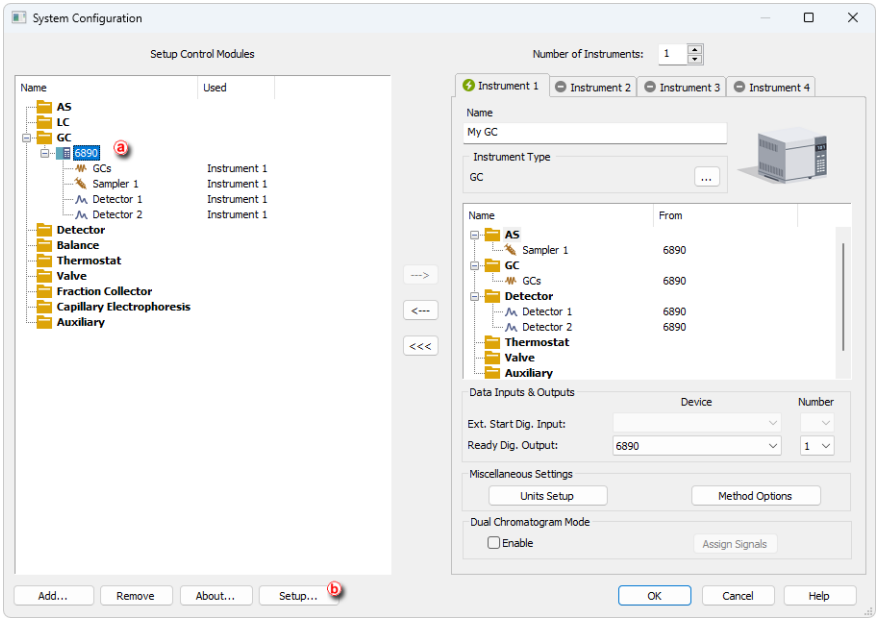
4. Add new devices to the appropriate instrument: drag and drop the device from the left pane ⓓ to the *Instrument* pane on the right ⓔ or select the device and click on `--->` ⓕ .



5. If you need to help with configuring a device, go to the topic ***Configuring a device***.

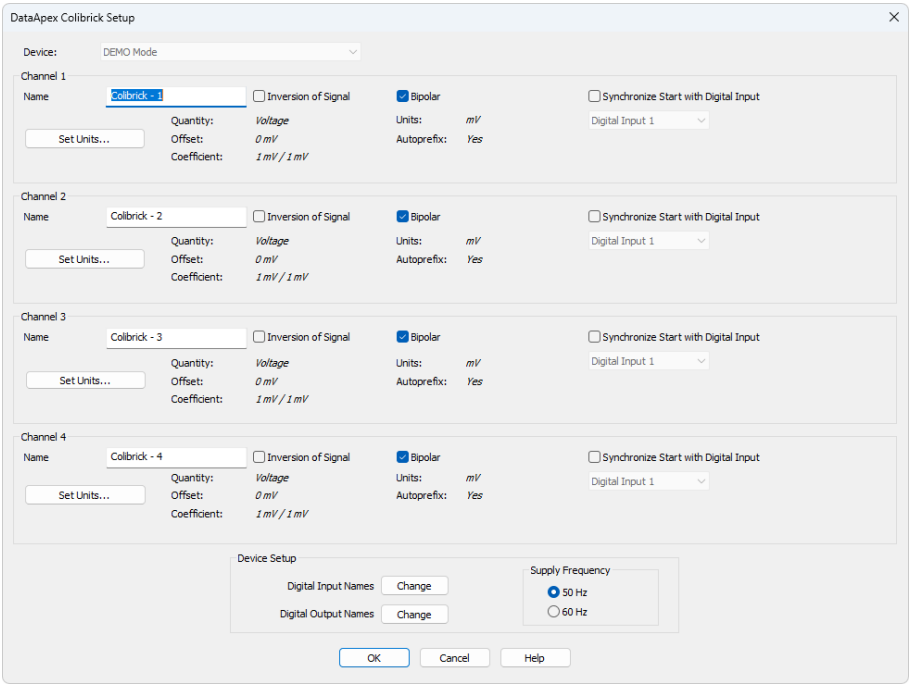
2.4 Configuring a device

1. Enter the *System Configuration* dialog: select *System - Configuration…* in the *Main* window.



2. To configure a device, double-click it or select it ⓐ and click the *Setup...* button ⓑ . A device setup dialog will appear. Setup dialogs are specific to each device.

For more information on how to configure a specific device, go to the specific manual or use the *Help* button.

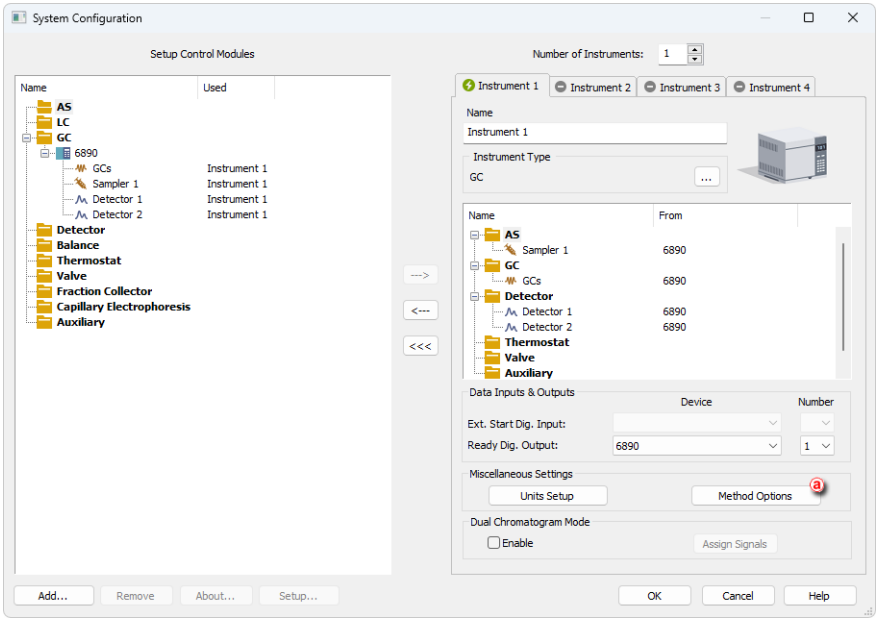


2.5 Setting the options for sending the method to the instrument

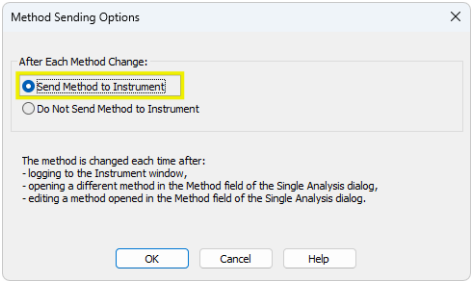
In a default Clarity installation, each time you change the method on Instrument, you need to send it manually to configured devices. Let's describe how to change that behavior so the method will be automatically sent to devices after each time you change the method.

Caution: We do not recommend to set the automatic sending of method on HPLC instruments since you may mistakenly send a method to configured pumps with wrong flow or pressure limits!

1. Enter the *System Configuration* dialog: select *System - Configuration…* on the *Main* window.
2. In the group *Miscellaneous Settings* click on *Method Options* button ⓐ .



3. Choose one of the option of the method sending.



If you select the *Send Method to Instrument* option, the method selected in *Single analysis* window will be sent every time you log into the instrument or this method is modified, or when the sequence is finished.

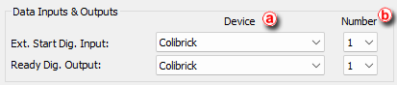
2.6 Assigning digital input and output to start acquisition

There are basically three means when Clarity decides to start the acquisition:

1. User presses Run button in Single Analysis (user probably did manual injection and notifies Clarity that its time to start)
2. Clarity is outside of run, but one of the controlled detectors starts to provide data marked as run data.

3. Clarity gets the digital input marked as START from device over:
    a. Communication line (LAN, serial (RS-232), USB/GPIB)
    b. Wire as TTL signal (this connection requires an external A/D converter or other device offering digital input to Clarity)

The last case (3) is most typical way and this chapter describes how to assign digital input and output in Clarity for the most common wiring of devices (typically an autosampler). The setting is performed in System Configuration dialog through *Ext. Start Dig. Input* and *Ready Dig. Output* functions.



2.6.1 Data Inputs & Outputs

- Settings are specific for each particular instrument.
- ⓐ : Only devices configured on the Instrument are offered in device list.
- ⓑ : Input number list allows to select input number. Available inputs are specific for particular instrument and correct number depends on actual wiring.

2.6.1.1 External Start Digital Input

The device (in most cases the sampler) provides the injection state to Clarity over its digital output. This may be a real digital output on the device or just a simulated one (Clarity does not distinguish between the two). Selecting a right *Ext. Start Dig. Input* is necessary, because Clarity watches the state of the selected input all the time and reacts on its change.

More Info:

Various devices are providing a lot of different inputs, and these may be used for other reasons, not only for analysis starting. The user needs to select the proper input which will allow the starting. For devices with virtual inputs, and in most cases also samplers with real outputs on the hardware, Start is signaled on output number 1.

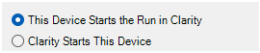
After receiving START signal from a sampler, that notifies Clarity about performed injection, Clarity sends instruction to Start Acquisition to other modules (detector, column oven etc.) of the system .

2.6.1.1.1 Possible synchronization issues

Missing start of analysis

Situation could happen when there is configured compact HPLC (without sampler) and external sampler or controlled sampling valve. The sampler or valve lets Clarity know, broadcasts the analysis start and the HPLC needs to get the information from Clarity, otherwise it will never start running.

For some chromatographs, the settings of the module and its behavior are set in the module's configuration based on the actual wiring, and it is upon the person installing Clarity and setting up the configuration to set the whole system correctly.



For correct option always consider the source of the analysis start first (sampler, sampling valve, Start button on a instrument) and ask a question "What will happen if Clarity does not signal anything? Will the instrument run anyway?"

- If **Yes** - option should be set to *This Device Starts the Run in Clarity*
- If **No** - option should be set to *Clarity Starts This Device*

2.6.1.2 Ready Digital Output

Note: Settings *Ready Dig. Output* in *System Configuration* dialog is relevant only for Active Sequence using sampler without **AS Control** module. Conversely is **not relevant** for controlled samplers used with **AS Control** module (signal over communication line), neither for Passive Sequence.

Ready Dig. Output defines the device and its specific pin through which Clarity informs other parts of the system that injection can be performed. After starting a sequence, controlled modules READY states are verified, Clarity triggers the *Ready Dig. Output* and changes its state, thus broadcasting to other modules of the system that sequence can be run. READY signal is received by the sampler that performs the injection and sends START signal. Then Clarity detects START signal and triggers again *Ready Dig. Output* and change its state, thus preventing the sampler to perform another injection.

Caution: Using the Event Table in Method Setup other actions can be configured changing the parameters of Digital Output. Note, that if the same Digital Output is modified, it may cause conflicts in synchronization. Avoid using these inputs and outputs in the Event Table.

2.6.1.3 Settings Examples

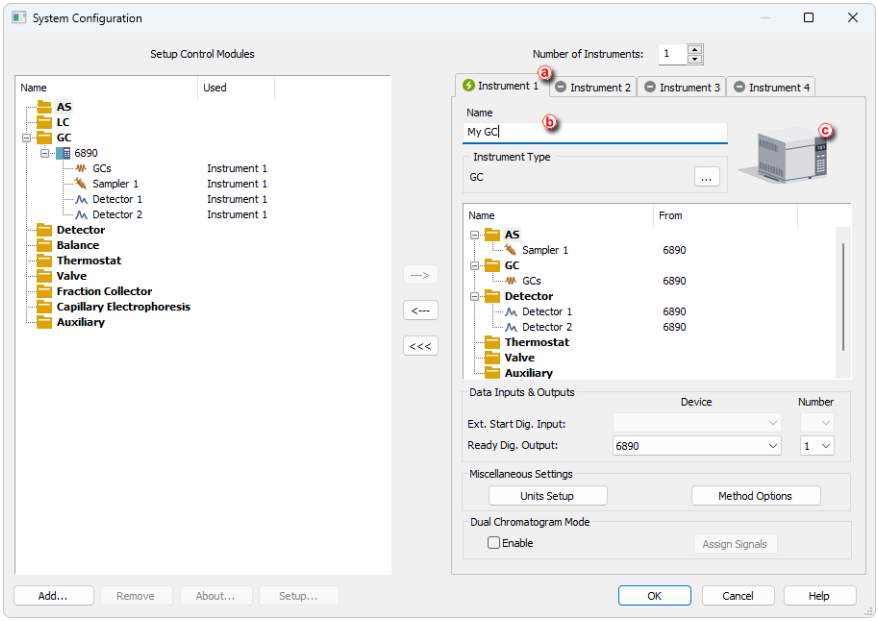
Default assignment of the *Ext. Start Dig. Input* and *Ready Dig. Output* functions can be found in the manual for the corresponding hardware.

For most common wiring of autosampler see chapter Connecting Autosamplers (AS) or respective subsections in **Getting Started manual**.

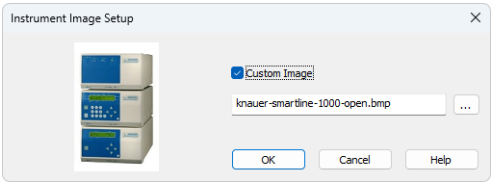
- AS + GC set - Active Sequence
- AS + LC set - Active Sequence
- AS + GC set - Passive Sequence
- AS with Clarity control module - Active Sequence + A/D converter
- AS with Clarity control module - Active Sequence + digital acquisition

2.7 Setting a custom image and a name for an instrument

1. Enter the *System Configuration* dialog: select *System - Configuration…*in the *Main* window.



2. Click on the *Instrument 1..4* tab to select the instrument ⓐ .
3. Type the name of the instrument in the *Name* field ⓑ .
4. Click on the image of the Instrument ⓒ to invoke *Instrument Image Setup* dialog.



5. Check the *Custom Image* check-box and then click on ... to select your image. Click *OK* to save your changes.
6. Repeat for every Instrument you wish to change the name or the pictures.

2.8 Tablet mode

This procedure shows how to activate and use a Tablet mode. The Tablet mode represents a specific windows layout that should simulate a single-window application. It is designed for devices with small displays. The optimum resolution is 1920 x 1080.

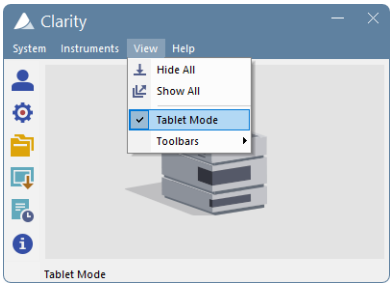
In Tablet mode, *Instrument window* is narrower than in standard layout and is positioned on the left side of the monitor, other windows open on top of each other and fill the remaining space on the monitor. Tablet mode allows the use of higher

scale in Windows (up to 200 %) which improves work with the software and readability of parameters.

Enabling Tablet mode

1. In *Clarity Main* window menu, click *View* and select *Tablet Mode* item.

   Note: Switching to Tablet mode is possible only when instruments are closed.



2. After logging in to the Instrument, new windows open in tablet layout. *Instrument window* is positioned to the left side of the monitor, other windows open on top of each other and fill the remaining space on the monitor.

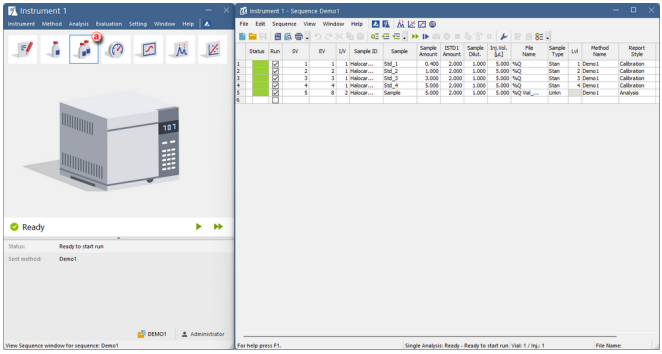
   More Info:

   Instrument window cannot be fully maximized. Its width can be expanded up to a maximum of 50% of the monitor width and is stored.

   Other windows always fill the remaining space of the display.

   Method Setup and *Single Analysis* windows are opened maximized.

   If the scale in Windows is set to more than 100%, some of the icons and analysis status line can break into a new line.



3. Icon of an active window is highlighted by a blue frame in the *Instrument window*ⓐ .

Disabling Tablet mode

1. In Clarity window menu, click *View* and select *Tablet Mode* item (active tablet mode is highlighted by a tick icon).
2. After logging in to the Clarity Instrument, new windows will open in layout used before activating the Tablet mode.

3 User Accounts

Chapters describing how to use User Accounts in **Clarity**, how to restrict some operations for defined users, and how to set shared settings for a group of users. User Accounts allow you to configure the settings for each user (Name, Password, Access Rights, and Digital Certificates) individually, and set the Password Policy for the whole station.

For the procedures on how to set the User Accounts to work in the GLP environment, see the *Clarity in Regulated Environment* manual.

The User Accounts can be configured from the *User Accounts* dialog. The proposed workflows regarding User Accounts are as follows:

3.1 Creating User Accounts

1. Open the *User Accounts* dialog: click on or choose *System - User Accounts*.
2. Create one typical *User Account*, that will be used as a template for others. More details can be found in the Creating a new user account topic.
3. Set the *Access Rights* of this user as needed. More details can be found in the Restricting Access topic.
4. Duplicate the created user account by the *Duplicate* command to copy the defined *Access Rights* to the new user. Set the *Name* and *Desktop file* of the new user. If needed, edit also the *Access Rights*. More details can be found in the Duplicating a user account topic.
    a. If you want the appearance of the tables, graphs, user settings, etc., shared between multiple users, set the desktop file to be the same for these users. More details can be found in the Sharing Settings topic.
5. Set the *Password Policy* to comply with your organization policy.
6. Save the *User Accounts* by clicking OK.

3.2 Managing User's Passwords

- When logging for the first time, or when the password expires, the user will be prompted to set a password during logging to Clarity. More details can be found in the Setting a password topic.
    - If it complies with the organization password policy, it is also possible to set a blank password. More details can be found in the Logging without password topic.
- It is also possible to change the user password any time you want. More details can be found in the Changing a password topic.

3.3 Managing User Accounts

- There are two ways how to terminate the User Account in Clarity.
    - Disable the user. The user account is still visible in the list in the User Accounts dialog, but cannot be used for logging in, nor changing its access rights. This is fully reversible as the user that has right to access

User Accounts dialog can *Enable* this account anytime. The user account with the same name as the disabled account cannot be created. More details can be found in the Disabling a user topic.

- Delete the user. After the saving the *User Accounts* dialog after deleting the user, this action is irreversible. The user account with the same name can be created. More details can be found in the Deleting a user topic.

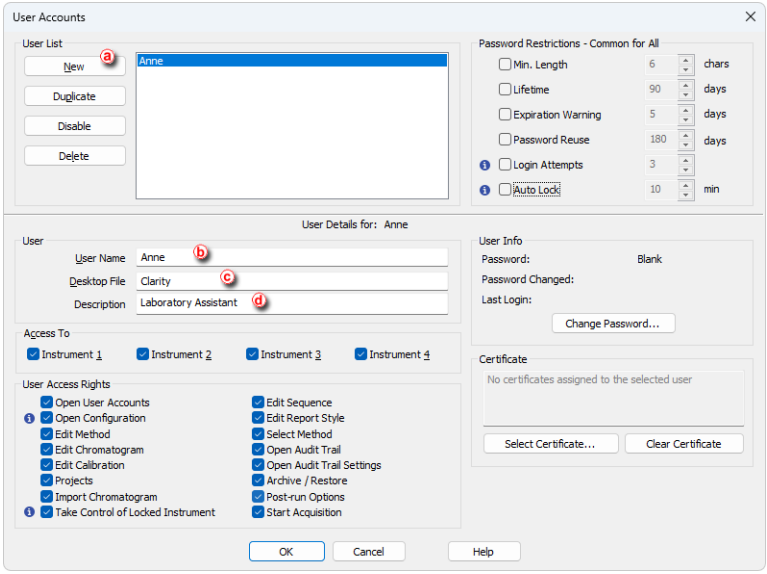
In the *GLP options*, it is possible to disallow the user account deletion and renaming, to ensure traceability and integrity of user accounts.

3.4 Creating a new user account

1. Open the *User Accounts* window: click on or choose *System - User Accounts*.
2. To create a new user, click the button *New* ⓐ and fill in the new *User Name* ⓑ .
3. Enter the *Desktop File* name ⓒ . If you left the *Desktop File* field empty, a [USERNAME].DSK desktop file will be automatically created.

   Note: This file contains settings regarding the size, location, and visibility of Clarity windows as well as all the modifiable Instrument parameters which are not part of system files.

4. Fill in a user *Description* if you want to. ⓓ
5. Click *OK* to accept the changes.

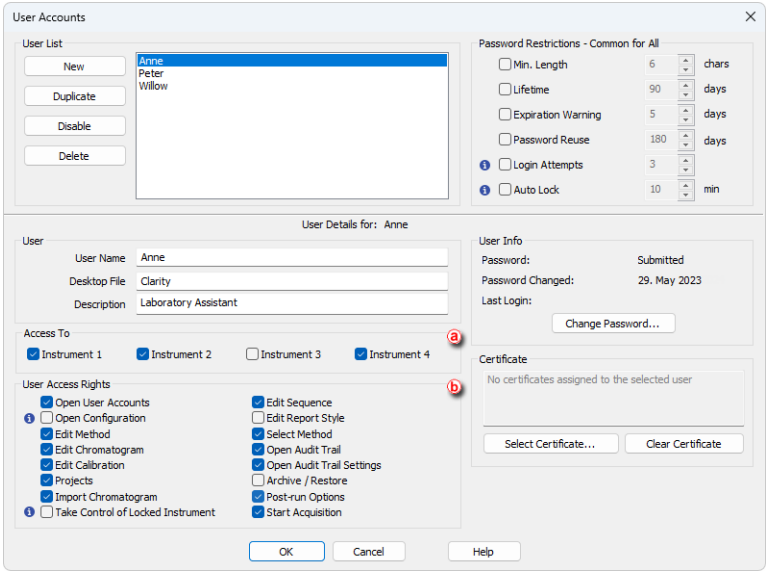


3.5 Restricting access

In Clarity, it is possible to:

- Restrict user's access to instruments
- Restrict user's access to Clarity procedures

1. Open the *User Accounts* dialog: click on or choose *System - User Accounts*.
2. Check the Instruments the user will have access to ⓐ .
3. Check the Clarity procedures the user will have access to ⓑ .
4. Click *OK* to accept the changes.

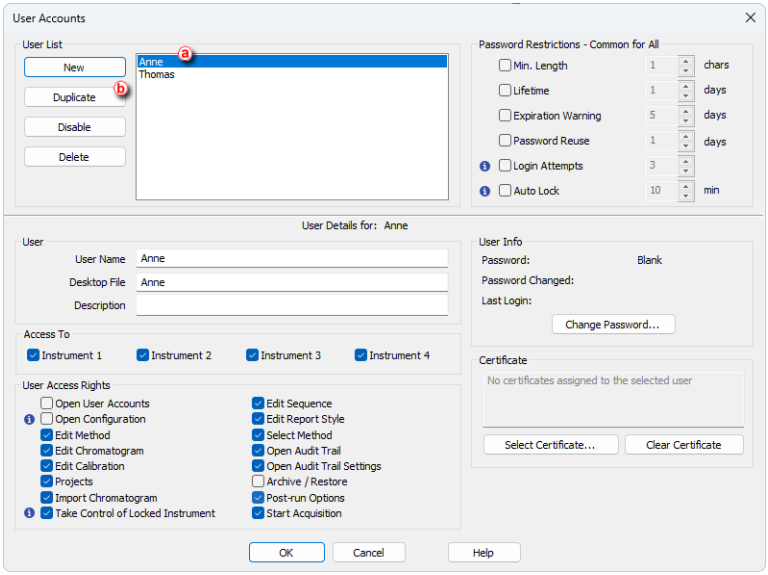


3.6 Duplicating a user account

Once you have set up the *Access Rights* for one account, it is possible to copy it to another new account using the *Duplicate* command.

To achieve this, follow these steps:

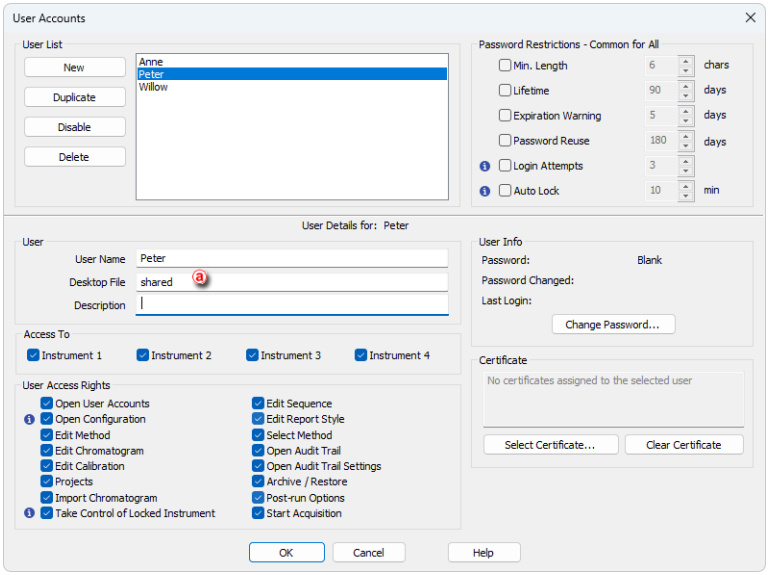
1. Open the *User Accounts* window: click on or choose *System - User Accounts*.
2. Select the account from which the settings will be duplicated ⓐ .
3. Select the *Duplicate* ⓑ command.
4. Enter the *User Name* of the newly created user account.



3.7 Sharing user settings among users

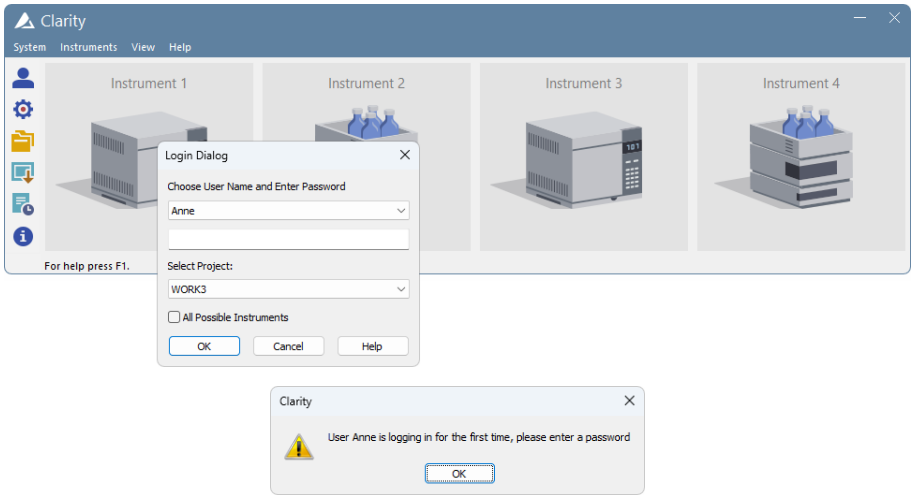
In Clarity, user settings e.g., settings of *User Columns*, the width of columns in tables, customization of toolbars, etc., are saved in the desktop files *.DSK.

1. Open the *User Accounts* dialog: click on or choose *System - User Accounts*.
2. Select the user to have a shared desktop file.
3. Type the name of the desktop file to be shared to the *Desktop File* field ⓐ .
4. Repeat the procedure for every user you want to have the shared desktop setting.
5. Click *OK* to accept the changes.

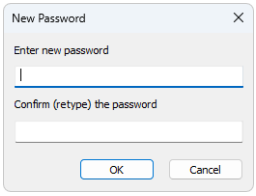


3.8 Setting a password for the first time

1. If the user has been created already and the password was left blank, then the first time you click on any of the instruments in the *Main* window, after selecting the user and clicking *OK* in the *Login Dialog*, you will be asked to enter a new password.



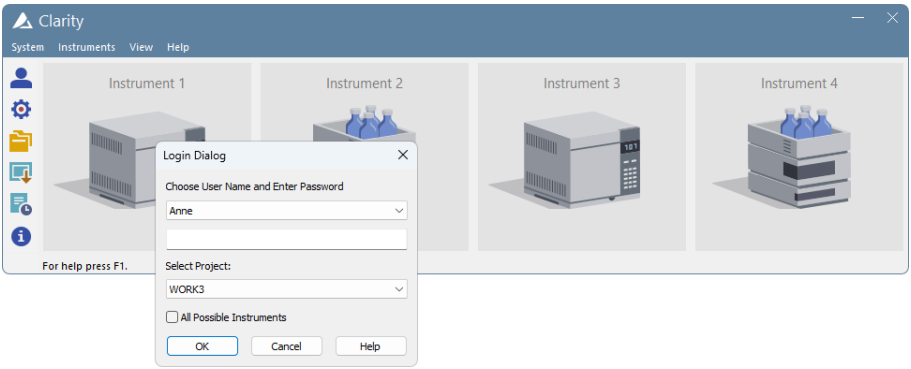
2. Type in and confirm the new password. Then click *OK*.



3. Alternatively or if you are creating a new user, you can follow the same procedure as explained in section *Changing a user password* and create a new one.

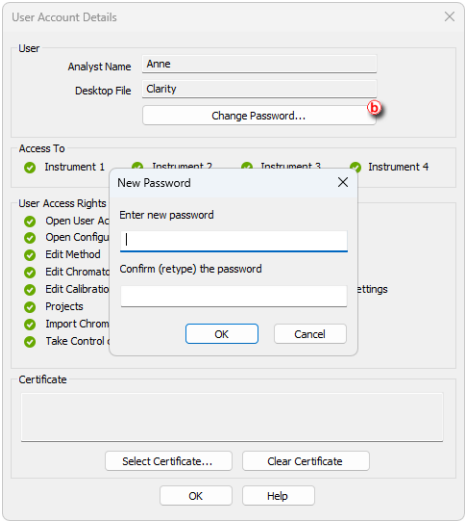
3.9 Logging in without a password

1. Create a new user account without setting up a password as explained in section *Creating a new user account* or remove the password, if it was previously set, in an previously created account as explained in *Changing a user password*.
2. Click on the *Instrument* you wish to open in the *Main* window.
3. Select the user name and click *OK* while leaving a blank password.



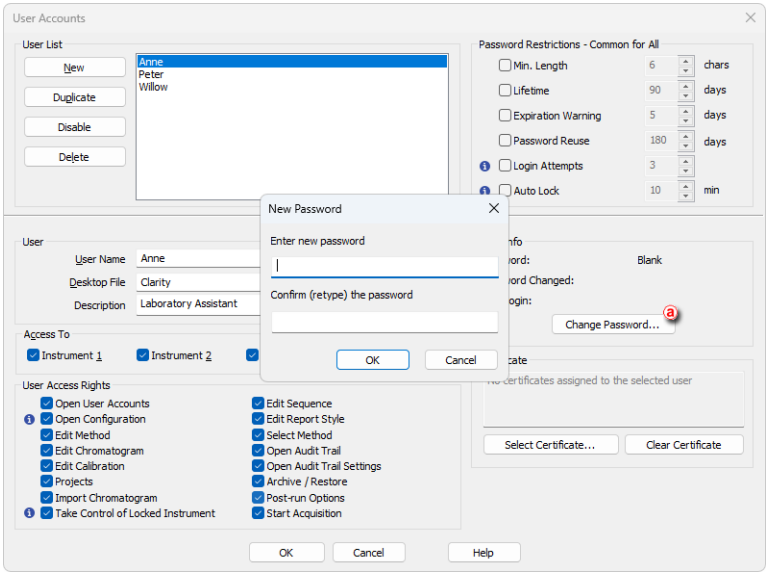
3.10 Changing a user password

1. Open the *User Accounts Details* window by choosing *System - User Details*, select the user, and enter the current password.
2. Click on the *Change Password* button ⓑ and enter and confirm the new password.



Alternatively, if you have access to the *User Accounts* dialog, you can change password by following these steps:

1. Open the *User Accounts* window: click on or choose *System - User Accounts*.
2. Select the user in the *User List* and then click *Change password* ⓐ .
3. Type the new password, confirm it, and click *OK*.

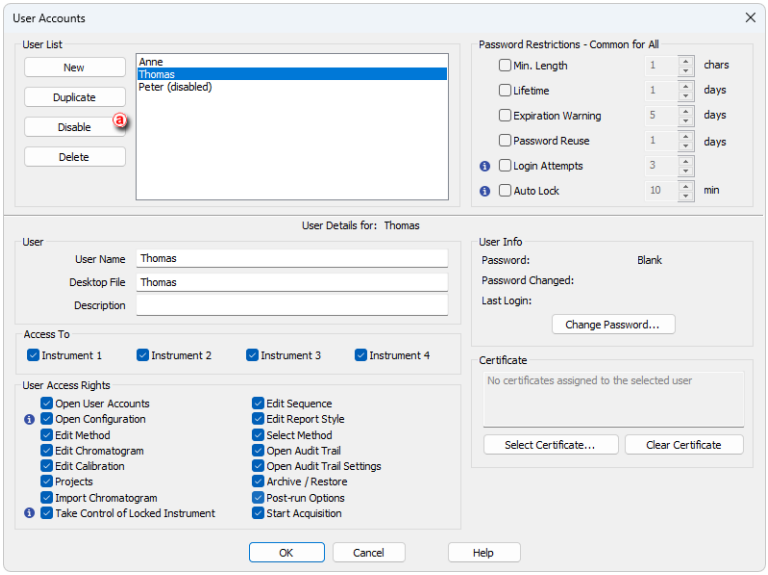


3.11 Disabling a user account

It is possible to disable a user account manually in the *User Accounts* dialog. Alternatively, accounts will get disabled automatically if *Login Attempts* are set, and the number of failed attempts was exceeded. It is not possible to log in to a disabled account, but it can be enabled again in the *User Accounts* dialog.

To disable or enable a user:

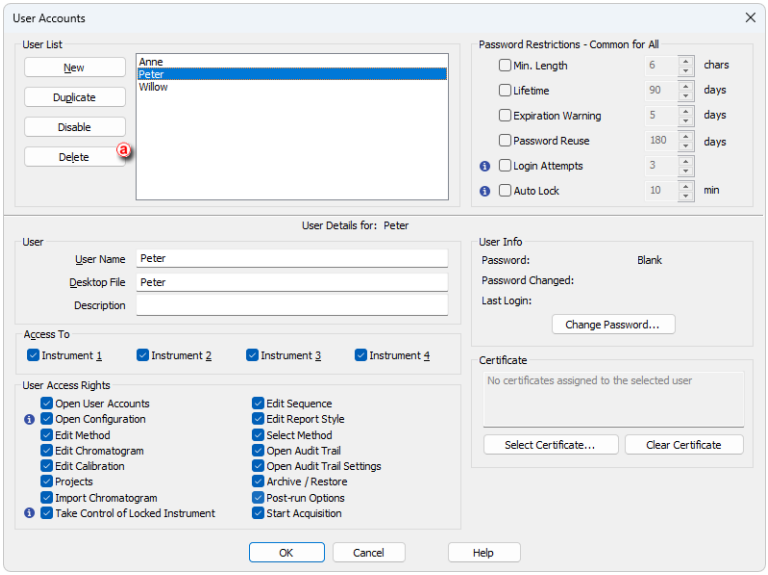
1. Open the *User Accounts* window: click on or choose *System - User Accounts*.
2. Select the user in the *User List* and then click the *Disable/Enable* button ⓐ .
3. Click the *OK* button to accept the changes.



3.12 Deleting a user account

1. Open the *User Accounts* window: click on or choose *System - User Accounts*.
2. To delete a user, select the user in the *User List* and then click the *Delete* button ⓐ .
3. Click the *OK* button to accept the changes.

Note: It is possible to disable the *Delete* function in the *GLP Options* dialog.


User Accounts
User List
New
Duplicate
Disable
Delete
Anne
Peter
Willow
Password Restrictions - Common for All
Min. Length
6
chars
Lifetime
90
days
Expiration Warning
5
days
Password Reuse
180
days
Login Attempts
3
Auto Lock
10
min
User Details for: Peter
User
User Name
Peter
Desktop File
Peter
Description
User Info
Password:
Blank
Password Changed:
Last Login:
Change Password...
Access To
Instrument 1
Instrument 2
Instrument 3
Instrument 4
Certificate
No certificates assigned to the selected user
Select Certificate...
Clear Certificate
User Access Rights
Open User Accounts
Open Configuration
Edit Method
Edit Chromatogram
Edit Calibration
Projects
Import Chromatogram
Take Control of Locked Instrument
Edit Sequence
Edit Report Style
Select Method
Open Audit Trail
Open Audit Trail Settings
Archive / Restore
Post-run Options
Start Acquisition
OK
Cancel
Help

4 Proposed workflow for routine analysis

Below there is description of a procedure that can be used for performing routine analysis of uniform samples. Steps are described in more details in linked topics.

1. Measure typical sample.
2. Adjust the integration of the chromatogram as needed. Details are described in How to integrate chromatogram topic.
3. Save the method including this adjusted integration. Details are described in Saving the chromatogram method as a template method topic.
4. Create model calibration that will be used in calibration cloning. Details are described in Creating model calibration to use in calibration cloning topic.
5. Set the calibration cloning in the sequence, method (and potentially in the calibration). Details are described in Calibrating using clone on first recalibration or Compensating for response drift using bracketing, Improving quantification with the standard addition method.
6. Create a sequence. Do not fill the levels of standard samples and post-run actions.
7. Run the sequence
8. Review the data. In case some minor adjustments are needed adjust the integration.
9. Fill in the Levels and post-run actions to the sequence file.

   Note: If you need to sign the documents and print the report with the signature, do not fill the Print actions in the sequence now. After the recalibration is performed, manually sign every chromatogram and then use Batch dialog - Post-run Options to print the reports with signatures.

10. In *Batch* dialog perform *Complete Processing* of the sequence. Details are described in Reprocessing whole sequence topic.
11. Now you have the sequence recalibrated, reports printed, and possibly other post-run actions performed.

5 Method Setup

Following chapters include useful tips regarding the *Method Setup* and working with method.

5.1 Setting up a method

The method essentially contains information on how the analysis will be performed, how the resulting signal will be processed and what events will be triggered and when.

Any method can be created or edited in the *Method Setup* window. To use the method for measurement it has to be sent to the instrument and for sequence measurement method has to be set at each row.

Template Method vs. Chromatogram Method

- The sent method is used as a template for new chromatograms and its contents are copied into the chromatogram file after acquisition or batch file reprocessing. You can open the different sections of the sent method setup from the icons in the *Instrument* window or with the command *Method - .....* on the toolbar.
- The changes to the chromatogram method do not affect the template method and they are performed in the lower pane of the *Chromatogram* window.
- The calibration file is linked to the template method and to the chromatogram method by its name.

Method Setup window

- The title of the *Method Setup* dialog displays a method that is currently opened. If you make any changes, the method becomes (MODIFIED).
- The upper part of the Method Setup dialog displays a set of icons with which it's possible to create a new method, open existing method, save method, save method as, open *Report Setup*, open method audit trail, send method by e-mail or open help.
- Upon pressing the OK button it will be automatically saved and *Method Setup* dialog will close.
- Tabs shown in Method Setup window are dependent on devices actually configured on the Instrument, e.g. MS Method, PDA Method, LC Gradient can be only visible when proper instrument type and device is set.

Send Method

- Only a method that is saved can be sent.
- Pressing the Send Method button will result in two actions:
  - Method will be sent to all connected hardware and thus displayed in the information table of the Instrument window - just as before.
  - Method will be set as Method for Single Analysis - you can start the single analysis form the instrument window using the icon.
- When measuring sequence, each row can have different method. It is set while creating or editing the sequence tab in the *Method Name* column.

Method Development

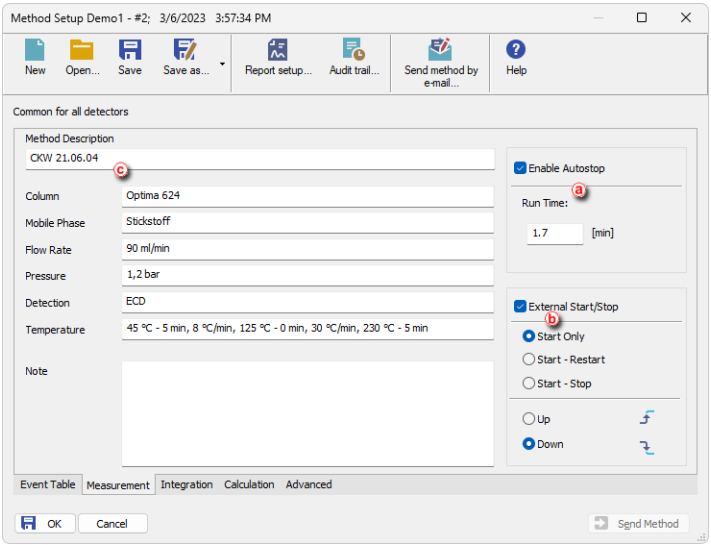
Method currently used for acquisition or present on already locked row of the sequence can't be edited, and can be viewed in read-only mode only.

When developing a method, you can configure the following settings among others:

1. **Set the measurement conditions.**

   Here you can disable or enable *Autostop* and set the run time for the analysis ⓐ as well as configure the external signal start and stop settings ⓑ (default setting *Start Only* should be used in majority of applications). *Autostop* can be set within interval 0.2 - 9999 min, such value is not influenced and does not influence any device specific time program settings on different tabs (like *LC Gradient* or *GC*). When time defined in *Autostop* passes, acquisition is finished, chromatogram is created, remaining time from time programs will be spent in so called *Control* state.

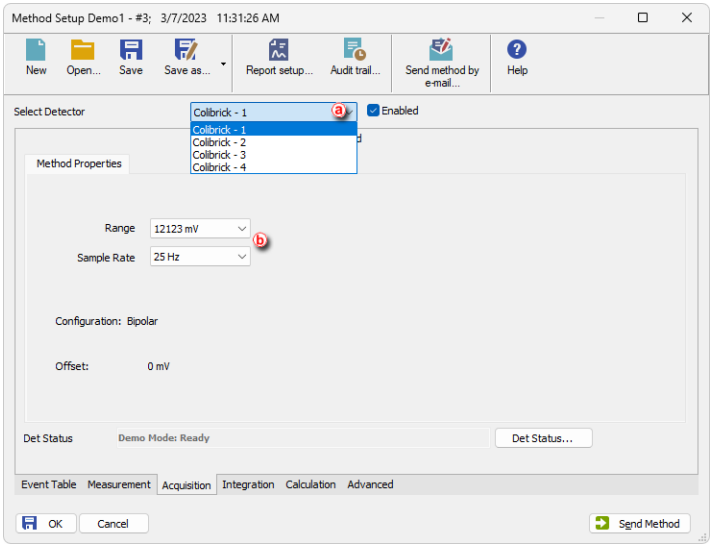
   You can also describe some parameters of the method and add a note ⓒ . Such information is purely informative and do not influence analysis in any way. They are saved into the resulting chromatogram and are showed in the *Chromatogram* window.



2. **Set the Data Acquisition parameters.**

   It allows you to select, enable/disable the detector signals ⓐ and to set measurement parameters e.g., the signal range and sample rate ⓑ . At any time at least one detector has to be *Enabled*.

   Layout of this tab, together with possible parameters to be set, are dependent on the configured devices (control modules) on the Instrument.

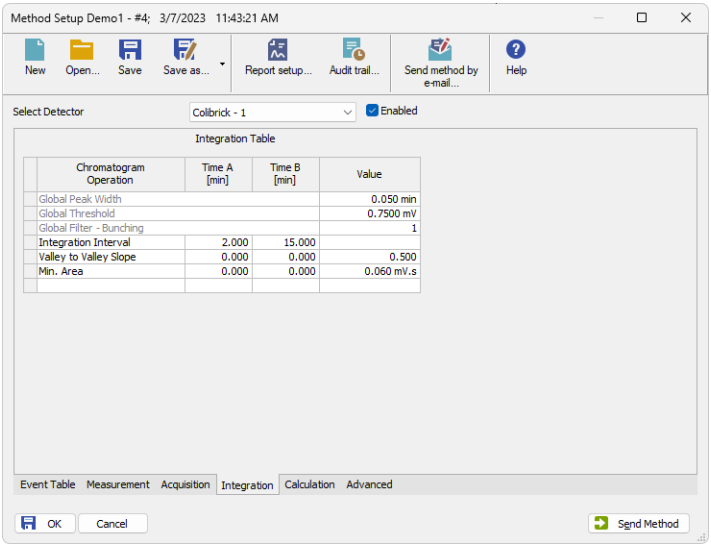


3. **Set the Signal Integration parameters.**

   When using a multi-detector configuration, there is an integration table for each detector (i.e. signal), thus every resulting signal can be integrated in a different way.

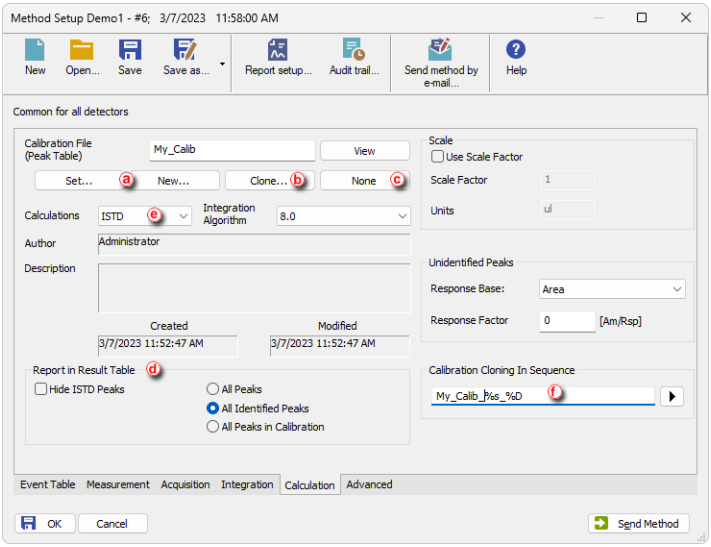
   Every resulting chromatogram acquired with such method will be integrated automatically accordingly the integration tab.

   If you aren't able to edit tab parameters the current detector probably isn't *Enabled*.



Note: Integration parameters are often modified manually after the first acquired chromatogram directly in the Chromatogram window. Then you can manually rewrite them into any method in the Method Setup dialog or you can use the *Method - Save as Template* menu command in the *Chromatogram* window to easily copy them into your method. For more details see the chapter **Saving the chromatogram method as a template method** on pg. **80**..

4. **Set the calculation options.**
   - You can create *New...* calibration file or *Set...* the one *created previously* ⓐ and configure the different settings related to it.
   - When calibration file is set, resulting chromatograms will be calibrated according to it and calibration standards will be used to automatically re-calibrate the attached calibration file.
   - *Clone...* ⓑ button will create a copy of a current calibration file. In the following *Save As* dialog you can select the name and location of the new calibration file. The copy will then be linked to the method.
   - If it is desired to have no calibration in the method you can use the *None* button ⓒ .
   - In this tab you can also choose how you want the results to appear in the results ⓓ and set calculation type ⓔ .
   - Name of calibration clone ⓕ must be set here to use calibration cloning in sequences, refer to chapter "Calibrating using clone on first recalibration" on page 112.



5. **Configure the settings in the additional tabs.**

   Method Setup also has tabs specific to currently configured devices and *Event Table* tab, used for configuring what events will be triggered and when e.g., shutting down Clarity after the sequence is finished.

   However, there are some limitations:

   - Event Table is for specific purposes, not needed for standard analyses.
   - Does not have control against infinite loops.
   - Must be filled per row, Fill Down/Fill Series can't be used in Event Table.

Note: For more information on any of the settings above, press F1 in such Clarity window to go the corresponding section of the Help or use the **Clarity Reference Guide**.

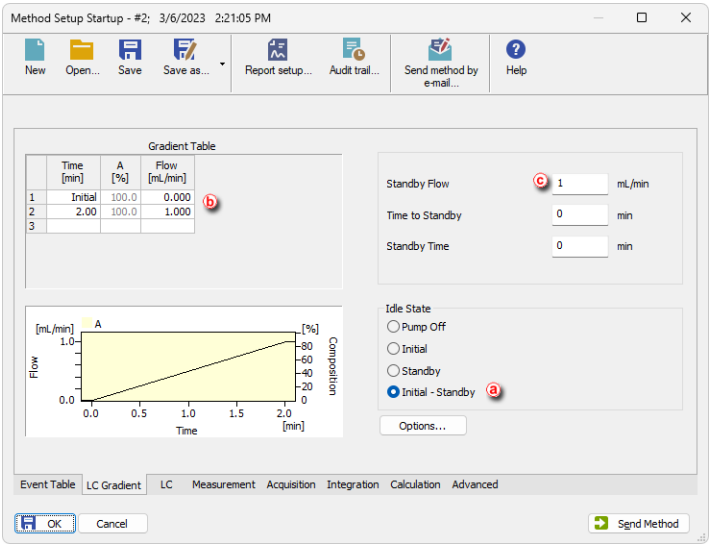
5.2 Setting up a slow flow rate increase and decrease on your LC pump

You can protect your chromatograph column from sudden pressure changes by setting up a *Sequence* together with three different methods, *Startup*, *Shutdown* and *Analysis* to ensure a slow flow rate increase and decrease on your LC pump. This procedure is mainly recommended for pumps controlled by Zebrick D/A converter or UNI Ruby scripts due to less strict pressure limit controls in these control types.

- Set the *Instrument Method Sending* option to "Do not send Method to Instrument", opposite to the topic *Automatic sending of a method to an instrument after each change*.

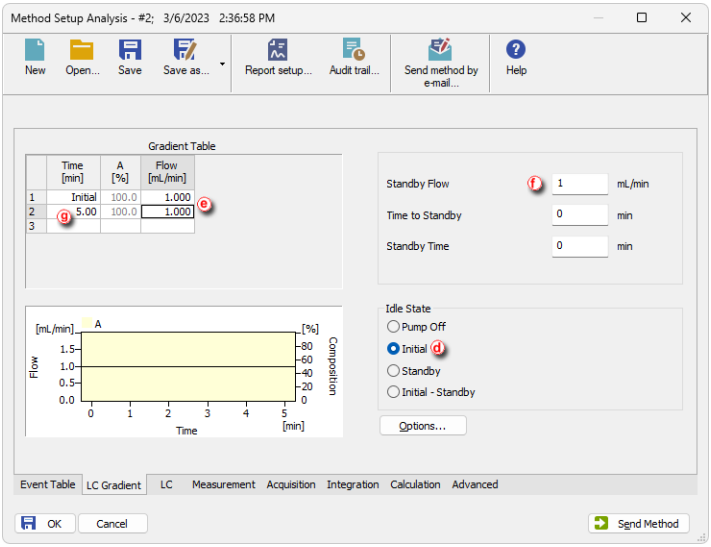
Startup Method

1. From the *Instrument* window open the *Method Setup* window using the *Method - Method Setup* command or the *Method Setup* icon.
2. Create *New Method* and *Save* it under the name *Startup*.
3. Navigate to the *Method Setup - LC Gradient* tab.
4. Set the *Idle State* to *Initial - Standby* ⓐ .
5. In the *Gradient Table*, ⓑ set the *Initial Flow* to 0 and on the second row set the *Flow* to its *Standby Flow* value ⓒ and the *Time* to obtain the appropriate flow rate increase for your column.
6. Click OK to accept the changes.



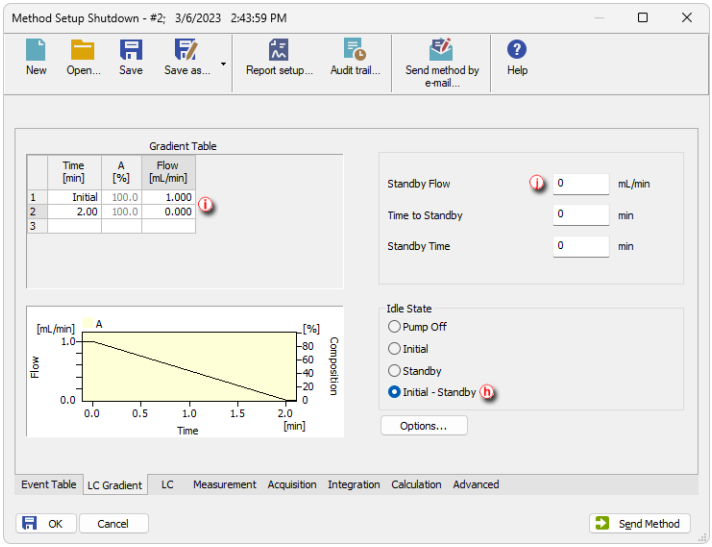
Analysis Method

7. Repeat steps 2 to 6 but this time:
   - Save the *Method* under the name *Analysis*.
   - Set the *Idle State* to *Initial* ⓓ .
   - Set the *Initial Flow*, *Flow* on the second row ⓔ and *Standby Flow* value ⓕ to the value of *Standby Flow* from *Startup* method.
   - Set the *Time* to the total duration of your analysis ⓖ .



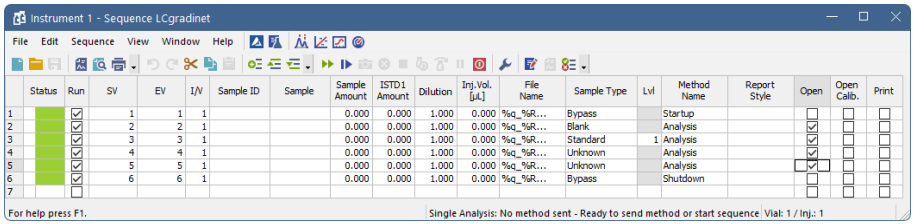
Shutdown Method

8. Repeat steps 2 to 6 but this time:
   - Save the *Method* under the name *Shutdown*.
   - Set the *Idle State* to *Initial - Standby* ⓗ .
   - On the second row, set the *Flow* to 0 and the *Time* to obtain the appropriate flow rate decrease for your column ⓘ .
   - Set the *Standby Flow* to 0 ⓙ .



Sequence

9. Set up a *Sequence* as explained in ***Running a Sequence*** and:
   - On the first row set the *Sample Type* column as *Bypass* and the *Method Name* to *Startup*.
   - On the last row set the *Sample Type* column as *Bypass* and the *Method Name* to *Shutdown*.
   - Set as many rows as you need in between according to the conditions of your analysis or sequence and set the *Method Name* to *Analysis*.



6 Event Table

The following chapters contain some useful tips on using the functions of the *Method Setup - Event Table*.

6.1 How to make a mark in a chromatogram during acquisition

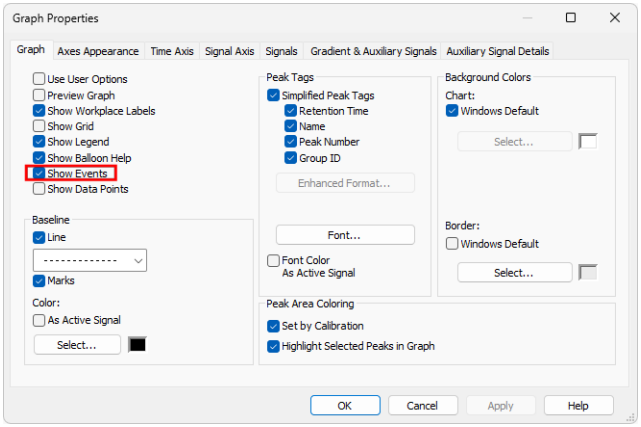
To create a mark in a chromatogram, you can use the *Event Table* tab from the *Method Setup* dialog and any hardware with digital input (such as Colibrick A/D converter) or the Virtual Digital Input Output Loop module. With the proper settings, triggering the digital input is recorded as an event, creating a mark (a vertical line labeled with name and RT) in the *Data Acquisition* and *Chromatogram* windows. The digital input can be triggered by pressing the start button when using HW or by pressing the corresponding Digital Output in the *Device Monitor* when using the Virtual Digital Input Output Loop module.

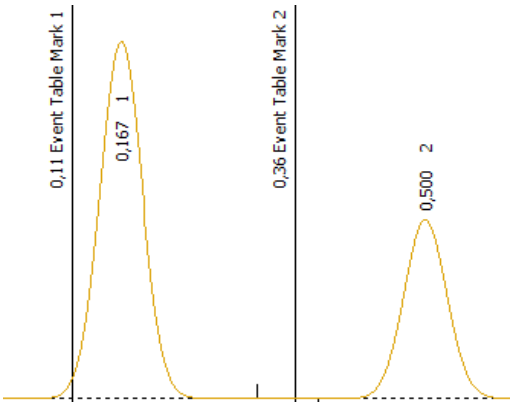
The following settings are necessary:

- HW with a digital input or the Virtual Digital Input Output Loop module configured to an Instrument.
- *Method Setup*
  - *Measurement* tab - *External Start/Stop* enabled and set to *Start Only*
  - *Event Table* tab - set according to the image below, where:
    - Name = the label of the event
    - Source = the module providing the digital input
    - Input = digital input recording the event

	Name	Input					Output			
		Type	Source	Input	Value	Units	Output Type	Output	Parameter	Store
1	Mark	Dig. Input Run	Colibrick	Digital Input 2	Down	---	None			☑
2										☐

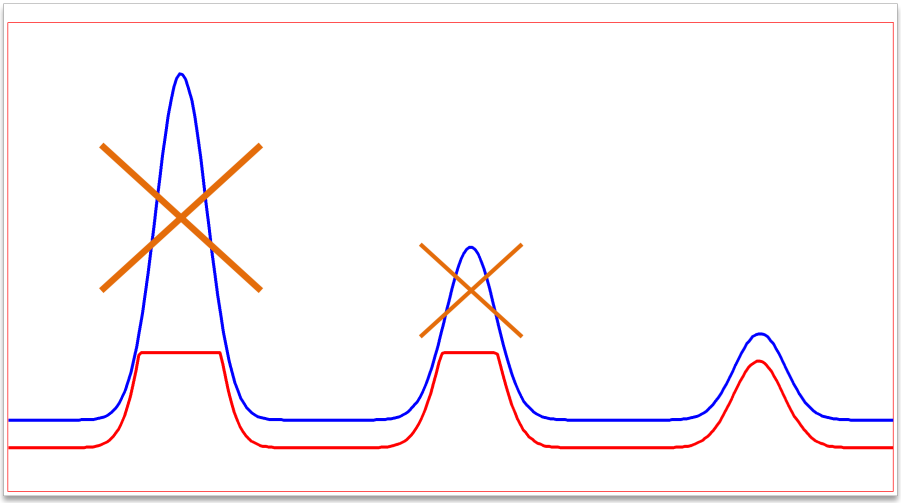
- To display the marks, enable the *Show Events* option in the *Graph Properties* dialog accessible from the *Data Acquisition* and *Chromatogram* windows (the dialog can be invoked by right-clicking the graph area in the respective window and clicking *Properties*...).





6.2 Signal out of range indication

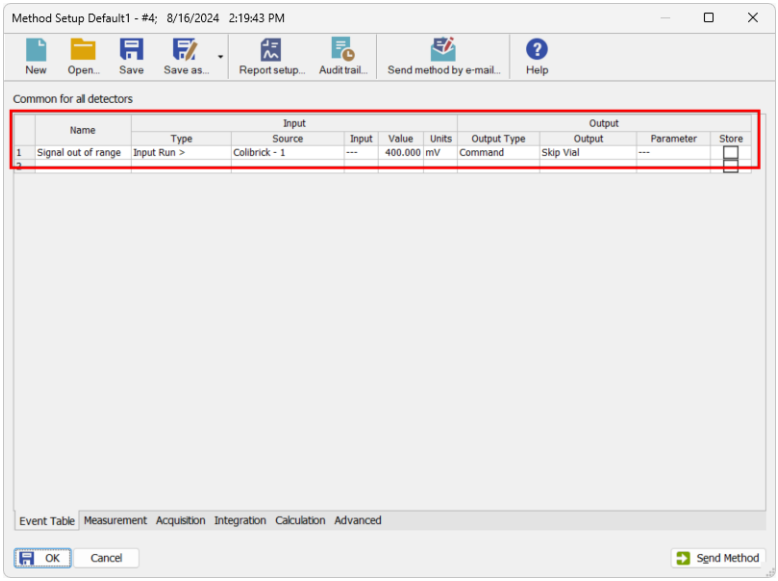
Under specific circumstances, it might occur that a portion of a peak is cut at top. This is caused by the signal being out of range of the current detector or A/D converter:



It is possible to indicate that a signal has reached a value out of the detector range via scheduling an event in the Event table. Such event needs to be triggered by the signal reaching a specific value, that is right below the detector maximum.

For that, set the event according to the following steps:

1. Open the *Method Setup* and prepare the method as necessary (or open an already existing method).
2. Switch to the *Event Table* tab.
3. Fill in the first row of the table:
   a. *Name* (e.g., Signal out of range)
   b. *Type - Input Run >*
   c. *Source* - your detector or A/D converter
   d. *Value* - slightly below the maximum range
   e. *Output Type* and *Output* - based on your requirements, for example *Abort*.



Once the entered input value is surpassed, the specified output event is triggered. Suitable output events also include alarm activation, close a contact, etc.

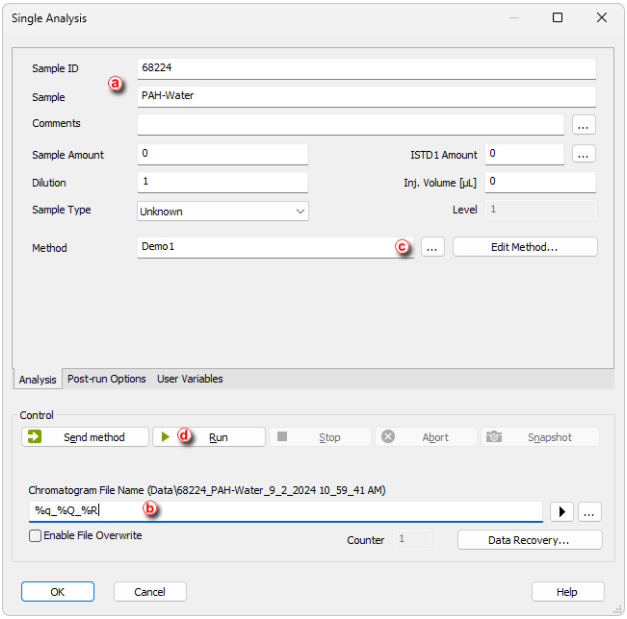
Note: Solvent peaks typically surpass the detector range. Consider the presence of a solvent peak in the sample before setting output events such as *Abort*, *Skip vial*, etc.

7 Data Acquisition

Chapters describing how to perform a measurement using *Single Analysis* or *Sequence* and how to evaluate chromatograms during run.

7.1 Running a single analysis

1. Open the *Single Analysis* dialog by selecting *Analysis - Single* or by clicking the icon in the *Instrument* window.
2. Fill in the sample information in the *Sample ID* and/or *Sample* fields ⓐ .
3. Fill in the *Chromatogram File Name* ⓑ . It is recommended to use variables to do so, for example, *%q* (*Sample ID*) and *%n* (counter) or *%R* (date and time) to prevent file name conflicts. Name preview is displayed above the field. For more info regarding variables see "Chromatogram File Name" in the Clarity Reference Guide.
4. Select the *Method* ⓒ which should be used for measurement. It is also possible to edit it by clicking *Edit Method*.
5. What should happen after analysis like automatic report printing can be set on the *Post-run Options* tab.



6. Start the analysis by clicking the *Run* button ⓓ . Analysis can be triggered also by an *External Start* from the chromatograph. The Instrument will switch to the

RUNNING state and the *Single Analysis* dialog will close. The state is visible in the status line of the *Instrument* window.

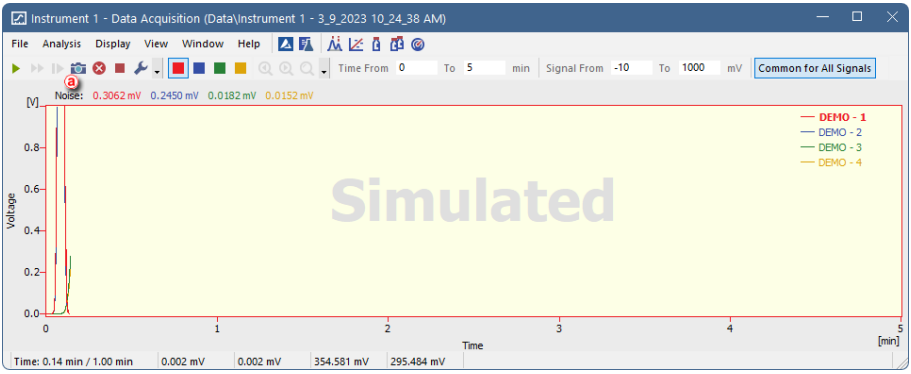
7. It is possible to monitor the analysis from the *Data Acquisition* window, see Pre-evaluating a chromatogram during acquisition for more information.

7.2 Pre-evaluating a chromatogram during acquisition

1. Open the *Data Acquisition* window by selecting the *Window - Data Acquisition* command or click the icon in the *Instrument* window.

2. To create a temporary chromatogram, select the *Analysis - Snapshot* option or click the icon ⓐ. Every time you take a snapshot, a temporary chromatogram will be created again from the analysis start up to the moment when you clicked.

Caution: To preserve a snapshot, it has to be saved under a new name. Otherwise it will be overwritten once the analysis is finished and the final chromatogram is created.



7.3 Creating and running a sequence

1. Open the *Sequence* window using the *Analysis - Sequence* command or the icon in the *Instrument* window.
2. Create a new sequence file using the icon ⓐ . or open an already existing sequence ⓑ . If you already have a sequence ready skip to step 12.
3. Save the new sequence using *File - Save As*…. Set the sequence file name and location in the *Save As* dialog.
4. Check the checkbox of the first (empty) row in the *Run* column ⓒ to add it to the sequence. The row will be pre-filled with default data, or with settings from the previous row.
5. Fill in the *Sample ID* and/or *Sample* columns ⓓ .

6. Fill in the *File Name* ⓔ . It is recommended to use variables to prevent file name conflicts, for example, *%q* (*Sample ID*), *%n* (counter), and *%R* (date and time). Hold the mouse pointer over the file name field to see the resulting name. For more information about variables, see "Chromatogram File Name" in the Clarity Reference Guide.
7. The *SV* (Starting Vial) and *EV* (End Vial) rows ⓕ will be pre-filled with numbers corresponding to the sample position in the autosampler tray, if you are using an autosampler. These can be changed as needed; it is also possible to inject from multiple vials in one sequence row.
8. Fill in the volume of the injection in the *Inj. Vol.* column ⓖ .
9. Select the method to be used for the measurement in the *Method Name* column.
10. Tick any of the *Open, Open Calib., Print* etc., columns ⓗ in case you wish to open the measured chromatogram in the *Chromatogram* or *Calibration* windows or print the results after each measurement of a sample.

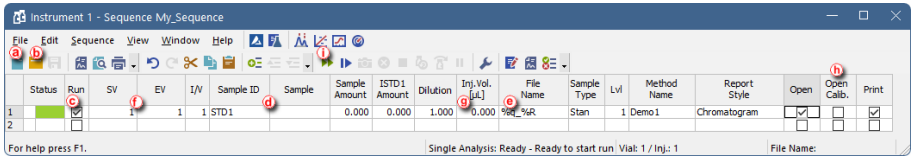
    Caution: To correctly include chromatographs in the reports, it is necessary to check both the *Open* and *Print* checkboxes. It is also necessary to fill in *Report Style* when *Print* or *Print to PDF* is used.

11. Repeat steps 4-10 for subsequent rows you need to add to the Sequence Table.

    Note: It is possible to display columns with additional parameters and post-run options by right-clicking the sequence table, selecting the *Setup Columns* command and moving items from the *Hide Columns* to the *Show Columns* list using the *Show* button.

12. Check the validity of the prepared sequence using *Sequence - Check Sequence* or by clicking the icon. In a valid sequence, all rows will show the mark in the *Status* column. Invalid sequences will issue a warning message describing the cause of the problem.
13. Save the sequence using *File - Save* or the icon.
14. Run the prepared sequence using *Sequence - Run* or the icon ⓘ .

    Note: The sequence state will change to the *WAITING FOR INJECTION* or *INJECTING* state, depending on the *READY* state of other controlled modules. The state is visible at the bottom of the *Sequence* window.



7.4 Editing the template for new sequences

Using the *File - New* command or the icon creates a new empty sequence. However, it is possible to edit the template from which new sequences are created.

As a result, a new sequence will already contain the pre-set parameters.

1. Open the *Sequence* window.
2. Use the *File - Open...* command or the icon to display the *Open Sequence* dialog.
3. In the *Open Sequence* dialog, navigate to the COMMON directory (click the icon), and open the TEMPLATE.SEQ file.

Note: There are analogous new sequence template files available for the EA Extension (EATEMPLATE.SEQ) and GPC Extension (GPCTEMPLATE.SEQ).

4. Set parameters in the new sequence template as necessary and save the file.

A new sequence created using the *File - New* command or the icon will contain the parameters as set in the TEMPLATE.SEQ file.

Caution: The sequence template files located in the COMMON directory are not project-specific, they are common to the whole **Clarity** station. It is however possible to set up custom locations of the Project directories for each *Instrument*. This includes having separate COMMON directories, and thus separate sequence template files. See the chapter **"Setting up project directories"** on pg. **191**. for more details.

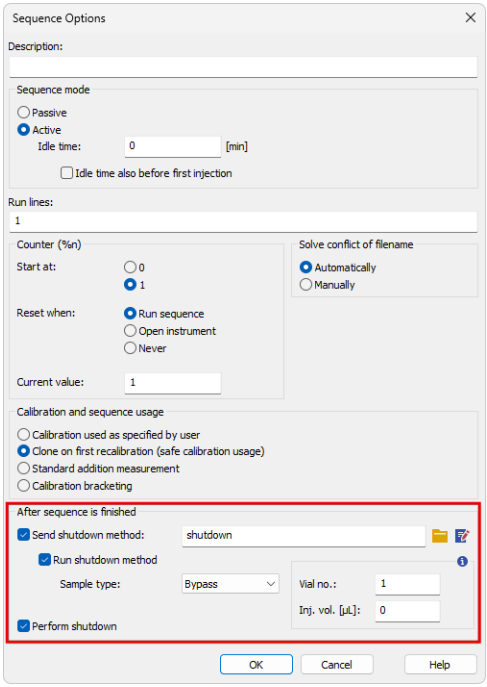
7.5 Shut down after finishing a sequence

After a sequence is finished, it might be convenient to send (and run) a shutdown method and/or perform shutdown. As the behavior of the used (controlled) devices may be quite specific, there are multiple options on how to get them to the desired standby state. For example, some detectors may be able to perform a run with lamps turned off or switch them off after end of a run, while others will not get to the *READY* state without the lamp on. A proper combination of the possible actions needs to be set accordingly.

1. To setup the shutdown parameters, open the *Sequence Options* in the current sequence using *Sequence - Options* or the icon.
2. Now, you need to decide whether you only need to send the shutdown method to the controlled devices to prepare them for the shutdown (step 3), or if you also need to run the selected method, e.g., for adjusting the gradient (steps 3 and 4). As mentioned in the beginning of this chapter, these settings are highly depended on the individual control module capabilities.
3. *Send shutdown method:* checkbox: Check this checkbox to send the selected shutdown method to the controlled devices. You can select or open/edit the method using the accompanying buttons. This option will only send the selected method to devices.
4. *Run shutdown method* checkbox: Use this option to run the selected method. The resulting chromatogram will be saved to the current project as [SEQUENCENAME - SHUTDOWN - METHODNAME - %R.PRM], where the %R variable stands for the current date and time.

Note: Use the sample type *Bypass* to omit injection from a vial, or *Unknown* for injection from a specified vial. Valid vial position and injection volume may be required by some autosamplers, even if the injection will not be performed (i.e., when the method is not run or the *Bypass* sample type is selected).

5. *Perform shutdown* checkbox: Use this option to shut down all controlled devices. The shutdown command is sent after completing the run of the shutdown method. Note that the reaction of some devices to the shutdown command may be adjusted in their respective *Setup* window in the *System Configuration*.



Note: The parameters of the *After sequence is finished* section are also executed when the user stops the sequence using the *Stop* command or when the sequence is stopped by an error. If it is necessary to stop the running sequence without sending (and running) the shutdown method, use the *Abort* command.

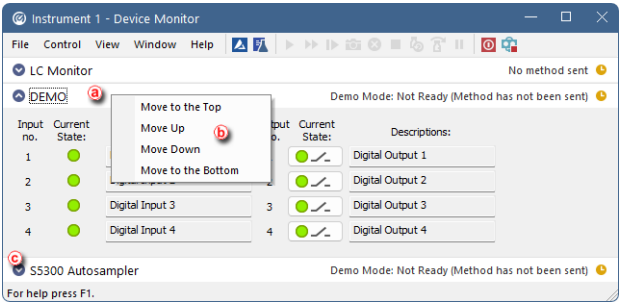
Note: When a sequence including the shutdown procedure is finished and new rows are added to the sequence, and such sequence is then resumed, the whole *After sequence is finished* will be applied again after the new rows are measured.

8 Device Monitor

The *Device Monitor* window serves firstly to show the current status of each control module and secondly for direct control of the device. The layout and possible control options greatly vary based on the used control modules.

The window can be personalized. To change the order of individual monitors right click on the module's name ⓐ and choose desired action in the *context menu* ⓑ .

The individual monitor panel can be collapsed or expanded using the arrow icon ⓒ in the header of the panel.

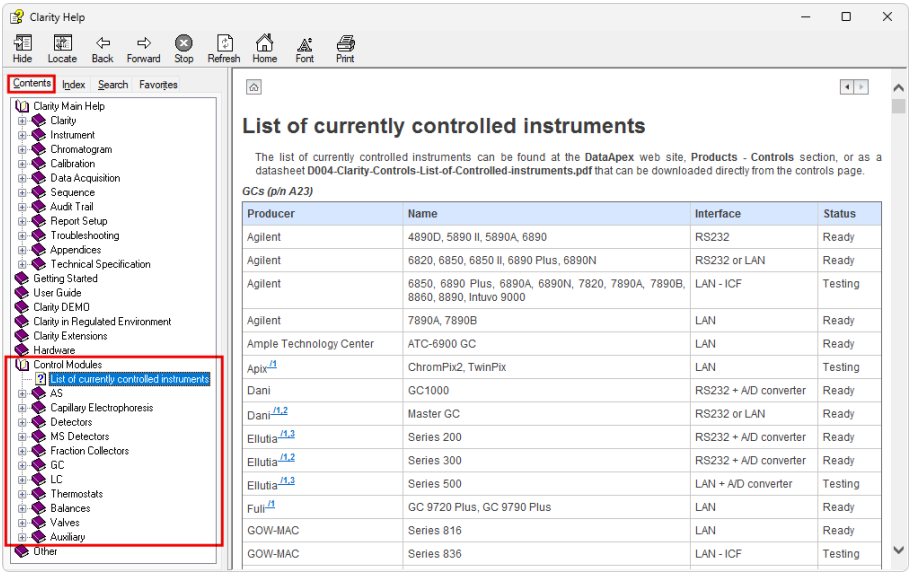


8.1 How to set parameters during run

Besides performing some service commands outside run, in some cases it is possible to perform some actions also during run. This is individual for specific control modules and could be found in the help or manual of respective control module. Control module helps are located at the bottom of the *Contents tab* of **Clarity** help which can be invoked by pressing *F1*. Manuals are available at www.dataapex.com/downloads.

Caution: Manuals are not available for all controlled devices. Control modules developed by third parties are only supplied with help file.

Common actions available for the pumps are described in next chapter.



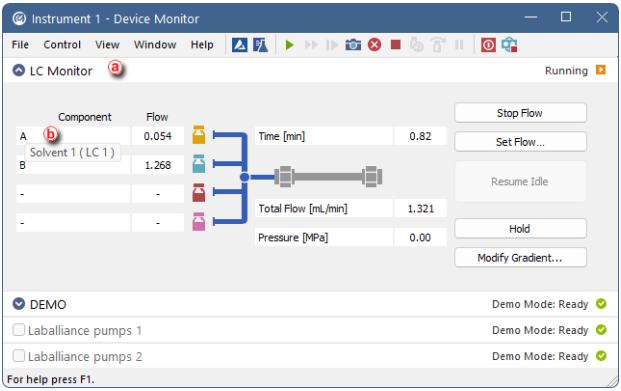
8.2 How to directly control LC gradient pumps during run

To control the configured LC pumps directly from **Clarity**, the *Device Monitor* contains the *LC Monitor* ⓐ section common to up to four pumps (i.e., a maximum of four solvents). Any combination of isocratic and gradient pumps can be used. If more than four pumps are needed, any additional pump has to be added as an auxiliary pump.

Note: The tooltip over each component shows the name of the pump ⓑ .

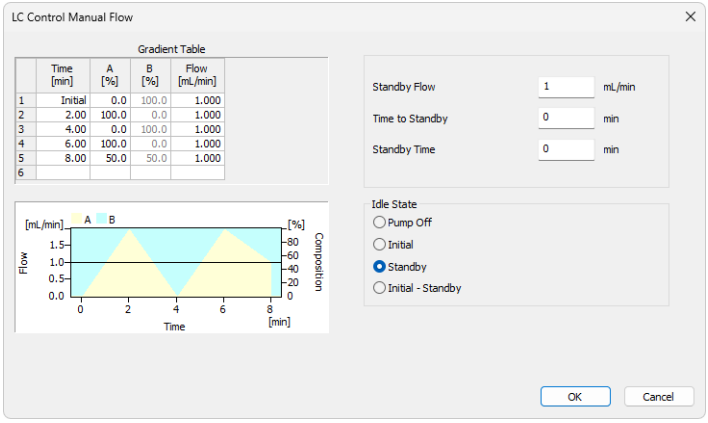
In the *LC Monitor* section of the *Device Monitor*, it is possible to:

- *Stop Flow* (the pump is stopped without stopping analysis) and *Set Flow* (a custom flow rate and composition can be set). Both of these buttons can be used outside or during analysis. Beware that when used during analysis, the gradient from the method cannot be restored and the set flow will be used for the rest of acquisition.
- *Resume Idle* switches the pump to the idle state as defined in *Method Setup - LC Gradient* tab.



Further commands are available for selected pumps (typically those controlled by **Clarity** in real time). They are enabled only during runs with a gradient program.

- *Hold* halts the gradient at its current state. The button changes to *Resume* which can be used to resume the gradient from the point where it was halted.
- *Modify Gradient* invokes the *LC Control Manual Flow* dialog (similar to the *Method Setup - LC Gradient*) which can be used to adjust the gradient for the current analysis. This does not influence the method used for analysis in any way.



9 Chromatogram Editing

This chapter focuses mainly on adjusting integration. For proposed general workflow see chapter How to integrate chromatogram

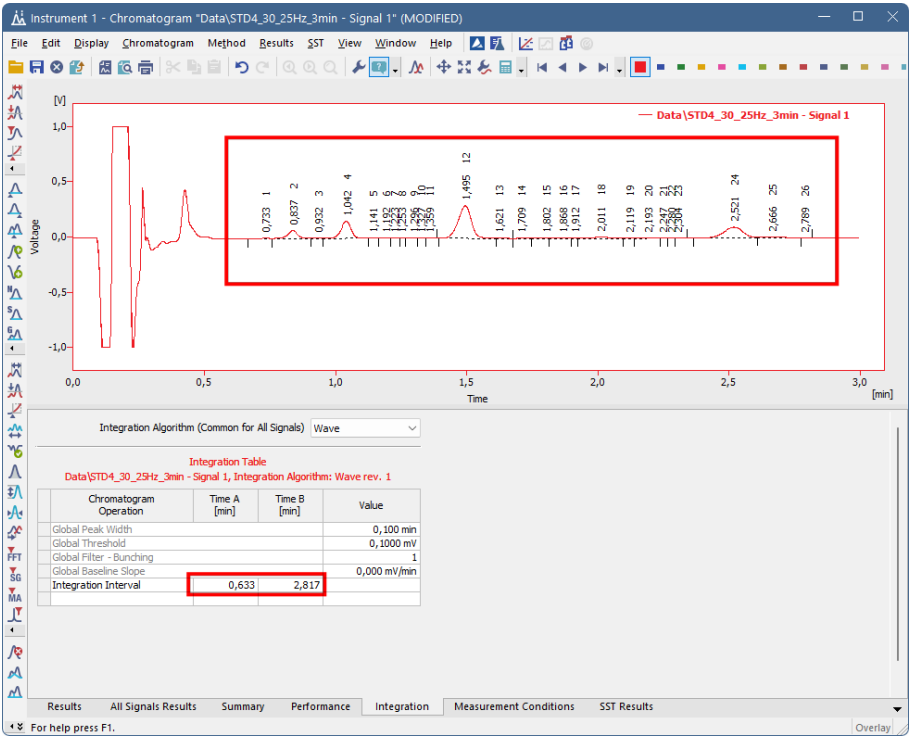
Clarity Tips&Tricks videos covering Integration topics can be found in Clarity Integration playlist.

9.1 How to integrate a chromatogram

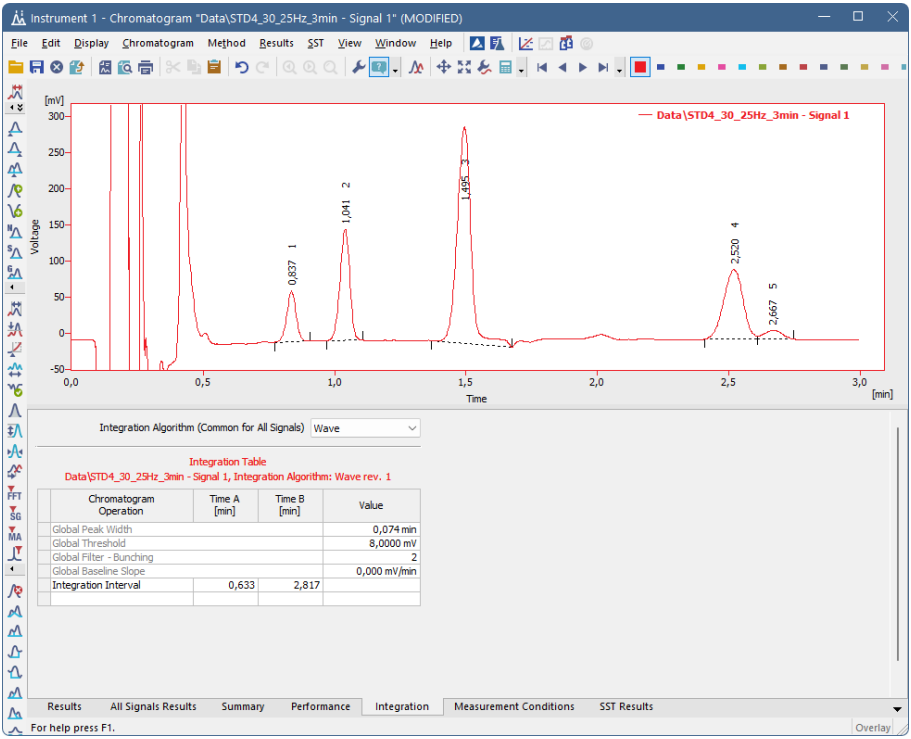
In order to automate the integration of routine samples as much as possible, it is necessary to optimize integration parameters and save them to the method used for measurements. Two integration algorithms (Wave and Legacy) are available, providing slightly different integration procedures. If you cannot achieve satisfactory integration using one of the algorithms, try using the other one. You can select which integration algorithm to use on the *Integration* tab of the *Method Setup* or *Chromatogram* windows.

1. Open one typical chromatogram for your analysis.

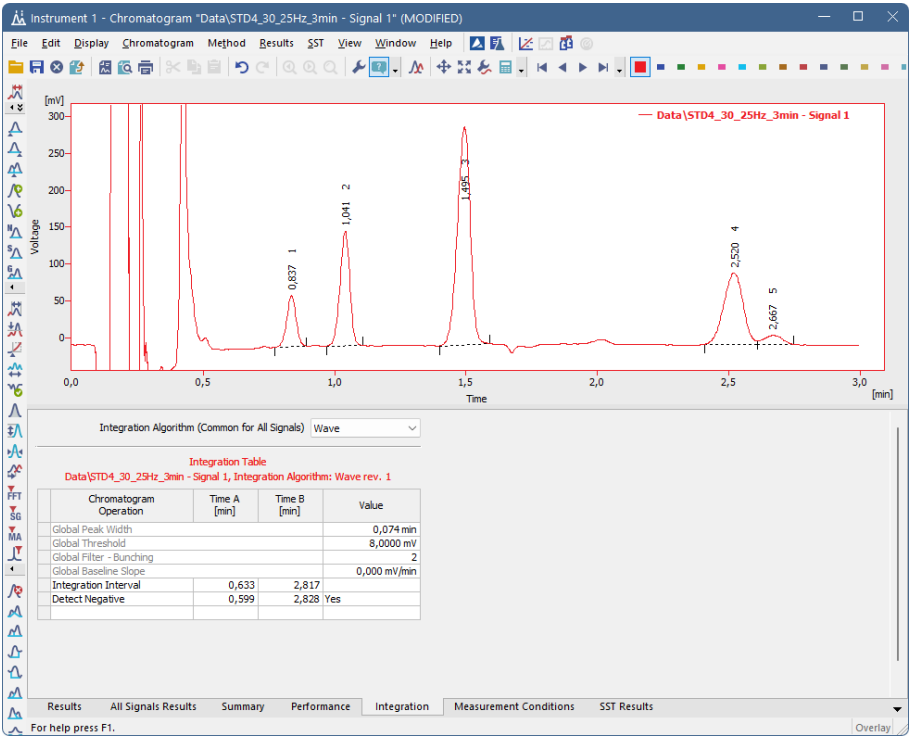
2. Set the *Integration Interval* as needed. More details can be found in the Setting Integration Interval topic.



3. Set the *Global Peak Width* parameter. Choose the narrowest peak which should be integrated in your chromatogram and select its start and end. This setting is used for calculation of *Global Filter - Bunching*.
4. Set the *Global Filter - Bunching* parameter. This is a filter which is calculated based on the *Global Peak Width* and sample rate.
    a. Alternatively, for chromatograms with a high noise, it is possible to use other filters - *FFT Filter*, *Savitzky-Golay Filter* or *Moving Average Filter*.
5. Set the *Global Threshold* parameter. This is influenced by the *Global Filter - Bunching* or other filter set previously. Select an interval containing only noise, not peaks. A more detailed description of the global parameters is covered by the topic Modifying Global parameters.

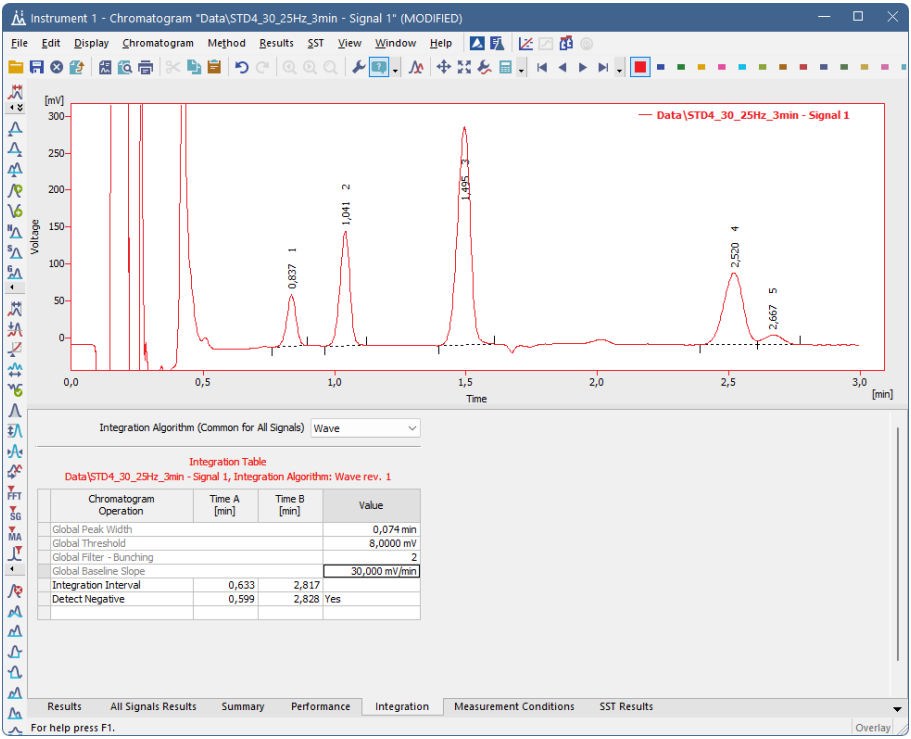


6. (Optional) Set the *Detect Negative* parameter. This setting has two potential uses: firstly, it can be used when you want to integrate negative peaks; secondly, it may help when the signal has inconsistencies such as dips. This will prevent the integration algorithm from placing peak starts/ends into them.



7. Set the *Global Baseline Slope* parameter. Change this parameter after you have all the peaks integrated, it servers to optimize their start/end positions.

Note: The *Global Baseline Slope* option is available only when using the Wave integration algorithm.



8. If you are still not satisfied with the integration, there are some other options for manual changes.
   a. Try to use some *Interval* parameters such as *Baseline Together*, *Baseline Valley*, *Forward Horizontal* etc..
   b. Or try to use some *Peak* parameters such as *Peak Start*, *Peak End*, *Peak Both*, *Add Positive* etc.

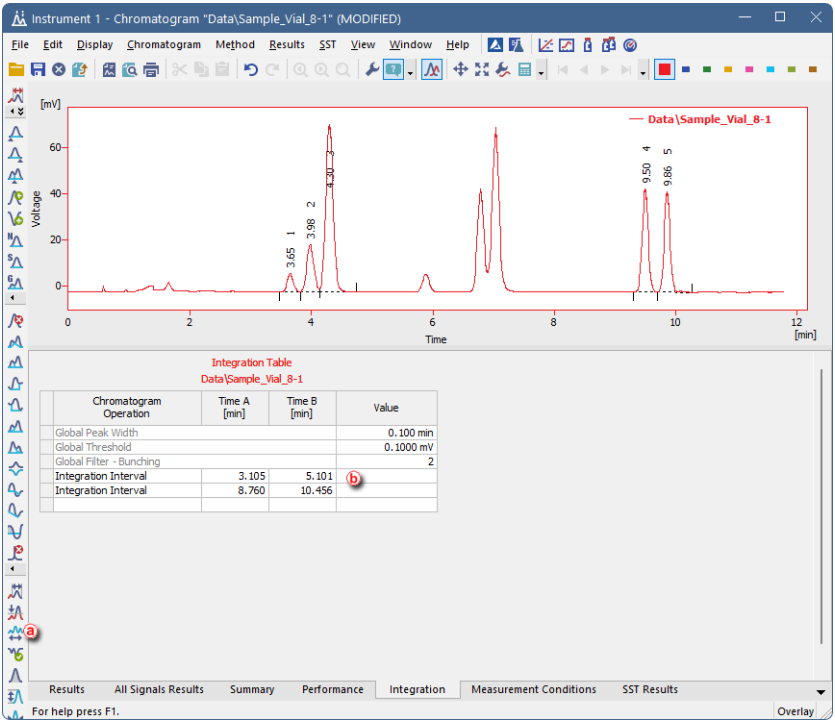
Note: The *Add Positive* operation should be used as the last resort because it is sensitive to retention time shifts. *Peak Start* and *Peak End* should be the preferred parameters as they are defined relative to peak apex.

9. When you are happy with the integration, you can Save method as Template and use it for further measurements of similar sample types.
10. If you have already measured some chromatograms and want to use these integration parameters on them you can do it using the Batch - Reprocess by Method.

9.1.1 Setting the integration interval

1. Signal outside of the interval is not integrated, this function is mainly useful for omitting solvent peaks etc.

2. To set the interval on which to apply the integration use *Chromatogram - Integration - Integration Interval* or icon ⓐ . It is possible to set multiple intervals within a single chromatogram.
3. You can check, modify the interval or delete this operations in the *Integration Table* ⓑ .



Note: If you want to exclude specific interval from the integration refer to ***Remove peak from integration***.

9.1.2 Modifying Global parameters

Peaks are only integrated if they exceed a minimum width (*Global Peak Width*) and height (*Global Threshold*). The *Global Baseline Slope* parameter influences the position of peak starts and ends. These parameters can be applied both globally or locally in a specified interval. It is always recommended to maximally utilize global parameters before using any local ones. *Global Filter - Bunching* works as a smoothing filter, it can to be applied only globally (to the whole chromatogram).

Global Peak Width:

- To adjust the minimum peak width use *Chromatogram - Global Peak Width* or the icon ⓐ and select the narrowest peak you want to integrate.

Global Threshold:

- To adjust the minimum peak height use *Chromatogram - Global Threshold* or the icon ⓐ and select an interval containing only noise, not peaks.

Global Filter - Bunching:

- Works as a smoothing filter that automatically averages number of data points in order to preserve at least 30 data points per narrowest peak. It is dependent on the *Global Peak Width* value. To use it, use *Chromatogram - Global Filter - Bunching* or the icon ⓐ after you are done adjusting the *Global Peak Width* parameter.

Global Baseline Slope:

- To adjust the minimum slope where the peak should start/end, use *Chromatogram - Global Baseline Slope* or the icon ⓐ and select the point where the peak should start/end.

Note: Available only in Wave Integration Algorithm.

If you are still not happy with the integration suggested by selection from the graph, you can manually modify the parameter values in the *Integration Table* ⓑ .

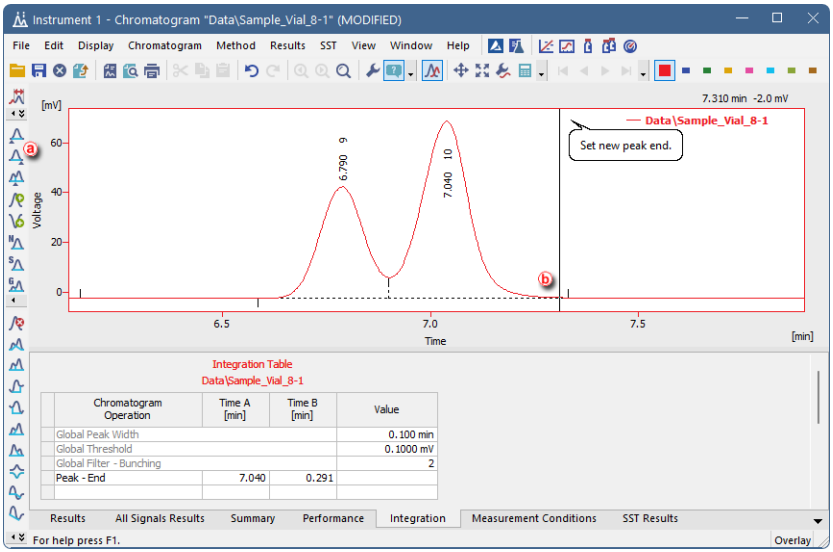
Setting the Local variants of Global parameters:

1. Setting local parameters is similar to the global ones, the only difference is that they are only applied on the selected time interval rather than the entire chromatogram.
2. To set a local parameter, use the *Chromatogram - Integration* context menu and select the parameter you need. Similarly, you can find the icon in the bottom part of the vertical toolbar ⓒ . Select the desired time interval in the graph. A small dialog appears ⓓ , where you can further specify the time interval and mainly select the value of the parameter. You can use the *Suggest Value* button ⓔ to select the value from the graph same as for a global parameter.
3. Again, all values can be further modified in the *Integration Table* if needed.

Note: *Global Filter - Bunching* is a filter that is always applied to the whole chromatogram. To filter data locally, use other filers from the *Chromatogram - Integration* menu.

9.1.3 Modifying the beginning and the end of a peak

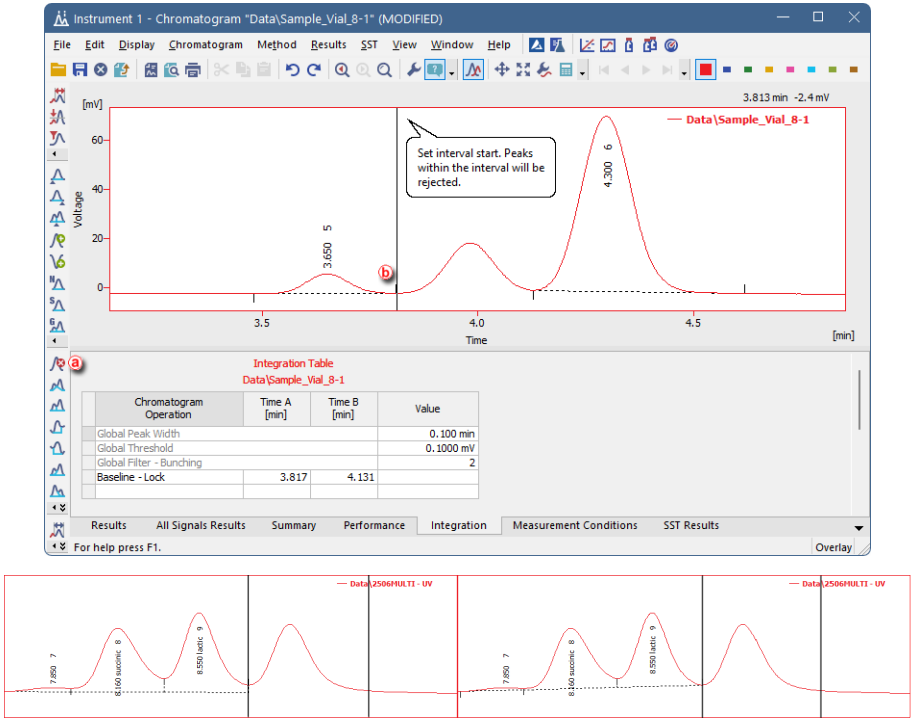
1. To change the position of peak beginning and/or end use *Chromatogram - Peak - Start* and/or *Chromatogram - Peak - End* alternatively use and/or icons ⓐ .
2. Set the new beginning ⓑ and/or end by clicking the new position in chromatogram graph.



9.1.4 Removing a peak from integration manually

With the introduction of the WAVE integration algorithm, there are now 2 ways to remove the peak from the integration. First one is present also in a Legacy Integration algorithm, the second is exclusive for the Wave IA.

1. Use *Chromatogram - Baseline - Lock* (or icon ⓐ) or *Chromatogram - Peak - Hide*.
2. Click once to mark the start of the interval that should be omitted from integration and click second time to mark its end ⓑ .



Difference between Peak Hide (left) and Baseline Lock (right).

Note the two vertical guidelines marking the beginning and end of the peak. More than one peak can be removed from integration at once.

9.1.4.1 Baseline - Lock

This tool completely removes all peaks that have their maxima within a set time interval. This could affect other peaks with maxima outside the specified window, particularly if they share the same baseline.

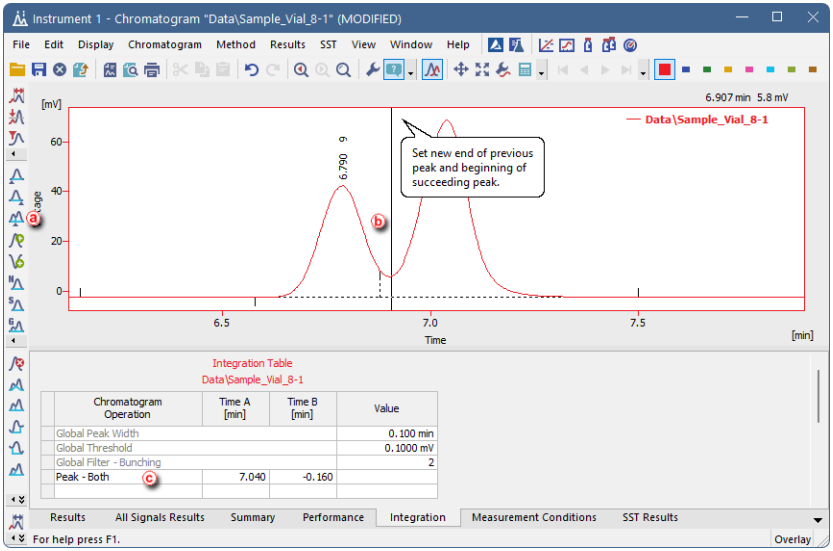
9.1.4.2 Peak - Hide (and Show)

By default, the Wave algorithm might automatically ignore some of the minor peaks identified during integration. However, completely eliminating these peaks could potentially affect the baseline's trajectory. Therefore, these functions offer a flexible way to handle unwanted peaks without completely removing them.

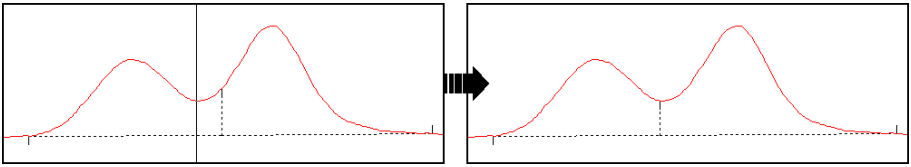
9.1.5 Changing the position of a peak separating line

1. Select *Chromatogram - Peak - Both* or click in the *Peak* toolbar ⓐ .
2. Set the new position of peak-separating line by clicking in the chromatogram graph ⓑ .

3. You can check, modify the position or delete this operation in the *Integration Table* ⓒ .

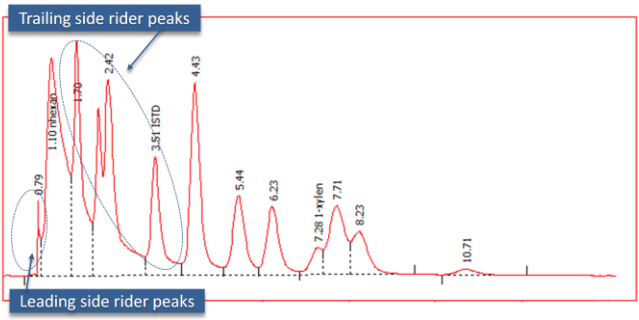


Note the vertical guideline indicating the currently selected peak separator position.



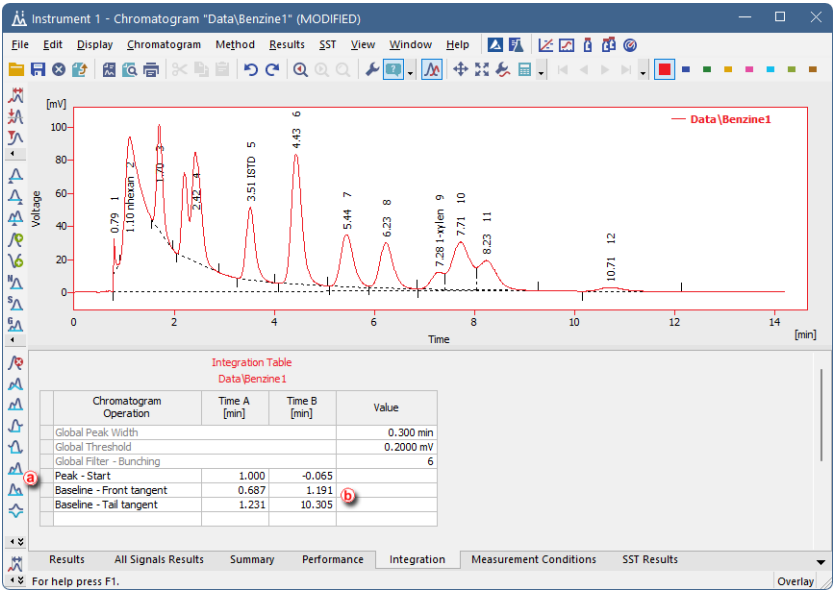
9.1.6 Separating rider peaks by tangent

Rider peaks are small peaks which are not well resolved from a large and asymmetrical neighbor but sit on its leading or trailing side.



1. Select the rider peaks you want to separate on the leading side of the mother peak: use *Chromatogram - Baseline - Front Tangent* or icon ⓐ .
2. Select the rider peaks you want to separate on the trailing side of the mother peak: use *Chromatogram - Baseline - Tail Tangent* or icon ⓐ .
3. You can check, modify the interval or delete this operations in the *Integration Table* (*Baseline - Front tangent* and *Baseline - Tail tangent* rows) ⓑ .

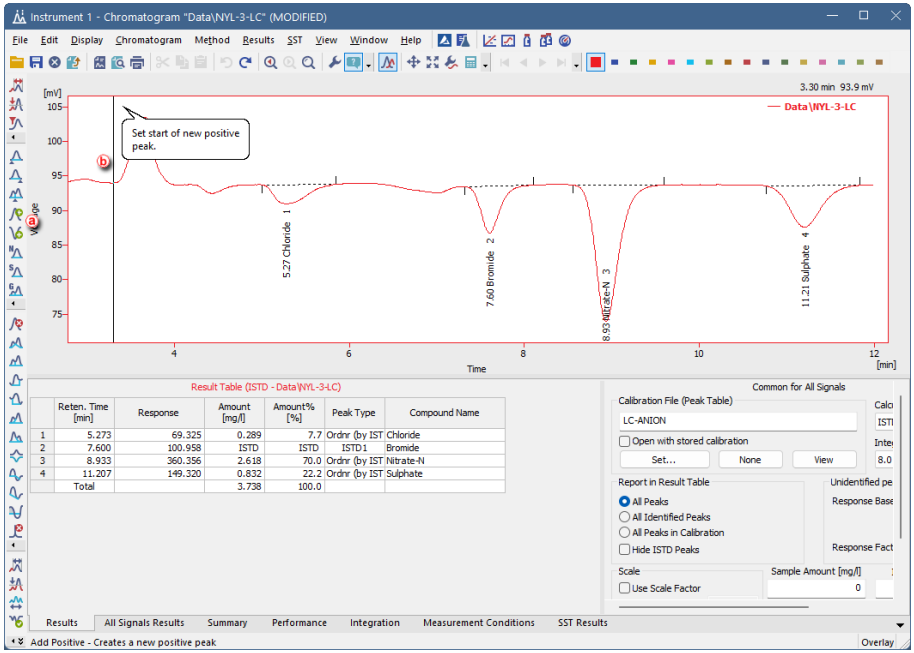
Note: You can also use the *Tangent Slope Ratio* and *Tangent Area Ratio* from *Chromatogram - Separation* menu to set a threshold for the separation of rider peaks based on those two parameters.



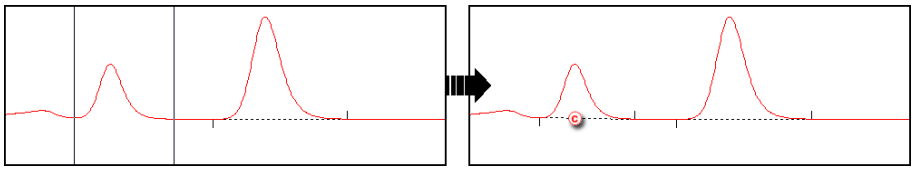
9.1.7 Adding a new peak manually

Caution: Manual addition of a peak should be used as a last resort to finish integration of individual chromatograms. Since the function is based on absolute time, when used in template method results might be inaccurate if retention time shift occurs.

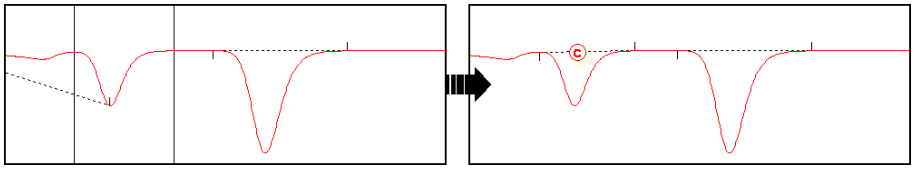
1. Select *Chromatogram - Peak - Add Positive/Negative* (also accessible from context menu) or click and in the *Peak* toolbar ⓐ . Holding Ctrl key while selecting the function will allow you to use it repeatedly.
2. Click in the chromatogram and set the beginning ⓑ and the end of a new peak.



Note the two vertical guidelines marking the beginning and end of the peak. After finishing the operation new peak is added ⓒ .



Add Positive

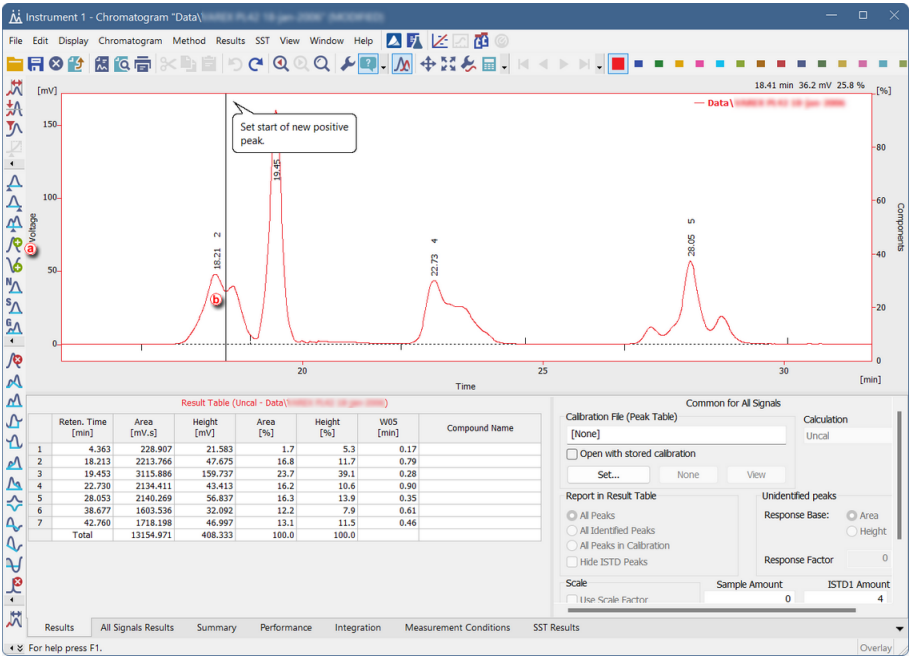


Add Negative

9.1.8 Splitting unresolved peaks using Add positive

The *Add positive* function can be also used for splitting unresolved peaks. Make sure to apply the function on the smaller part of the unresolved peak.

1. Select *Chromatogram - Peak - Add Positive* (also accessible from context menu) or click in the *Peak* toolbar ⓐ .
2. Click in the chromatogram and set the beginning ⓑ and the end of the smaller part of an unresolved peak.



A vertical guideline will appear dividing the unresolved peak.

9.2 Saving the chromatogram method as a template method

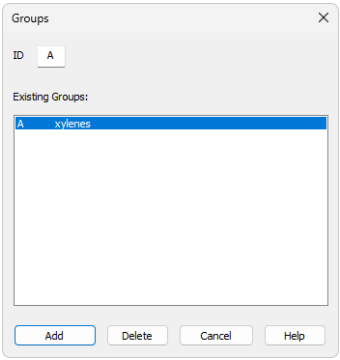
Each chromatogram contains saved copy of the method used for acquisition of such chromatogram. However, changes done in *Chromatogram* window (e.g. *Description, Integration Parameters, linked Calibration File*...) are not updated in the original method used for acquisition nor processing. To amend your method accordingly, you can create template method from the method in chromatogram, which is useful after optimizing integration parameters.

1. Open the chromatogram with optimized method.
2. Select the *Method - Save as Template…* to save the method (including the changes made by you) from the current chromatogram as a new method, or for example overwrite (update) your acquisition method.

Note: It is not possible to overwrite any method that is currently in use, for example a method opened on any Instrument.

9.3 Adding a peak to a group

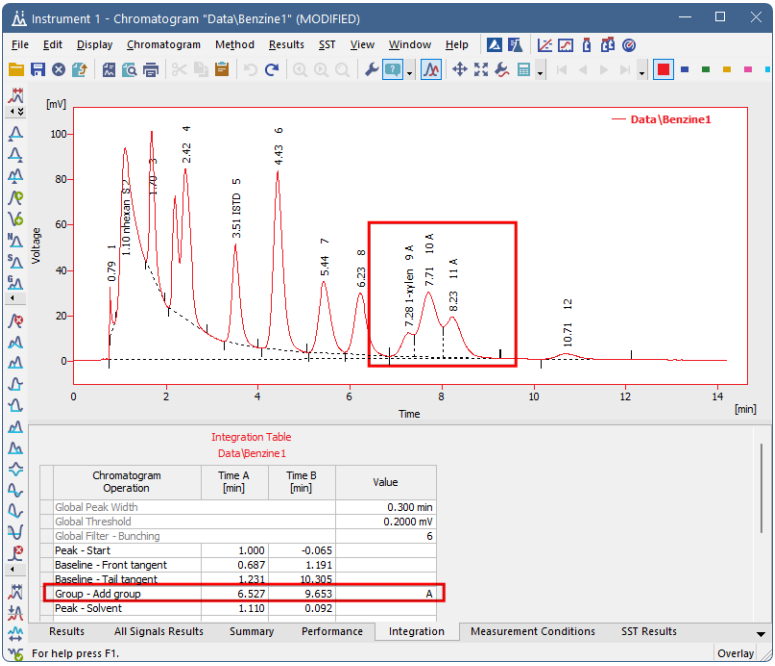
1. Use menu item *Chromatogram - Peak - Peak Groups…* to invoke *Groups* dialog.



2. Either select an existing group from the list or create a new one by inserting a letter to *ID* (groups are defined by a single letter) field and click the *Add* button.

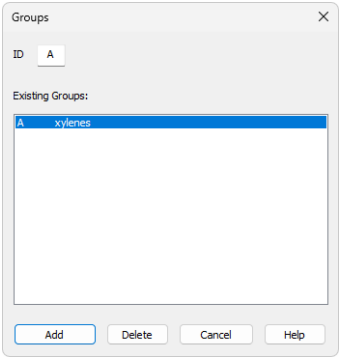
   Note: Group Name is based on the calibration file, similarly to the Compound Name.

3. Click in the chromatogram for the first time to select the start point and second time to select the end point of the group interval. Peaks with apexes found in the interval will be added to the new group.

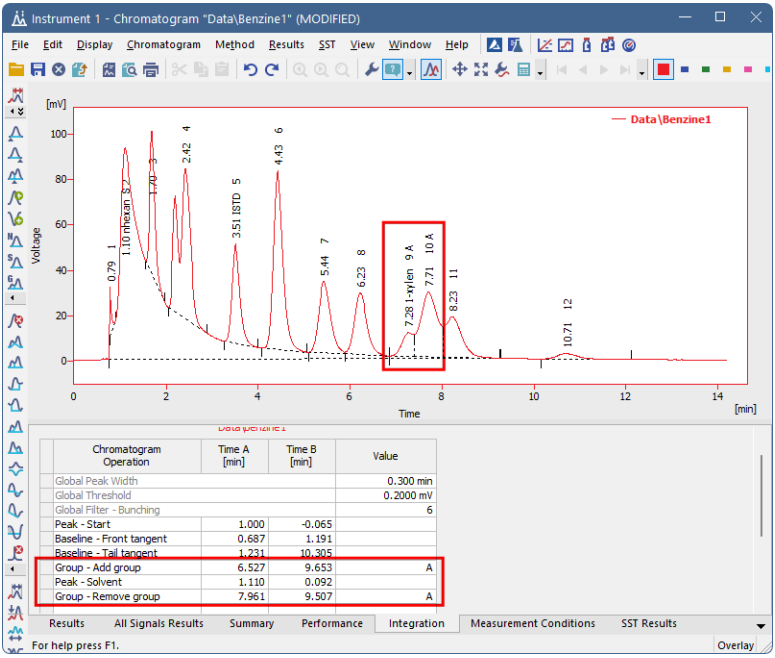


9.4 Removing a peak from a group

1. Use menu item *Chromatogram - Peak - Peak Groups…* to invoke *Groups* dialog.



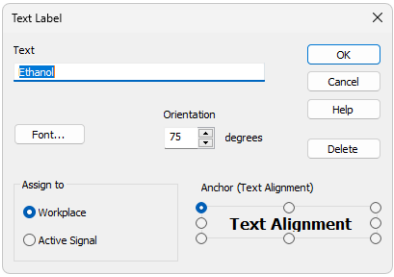
2. Select an existing group from the list and click *Delete*.
3. Click in the chromatogram to select the start and again to select the end of the interval which should be removed from the group.



9.5 Adding text and lines to a chromatogram

Adding text label

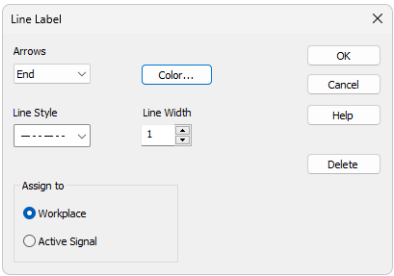
1. Right-click in the chromatogram graph to invoke context menu and select *Create Label - Text*.
2. "T" will appear next to the cursor, click wherever you would like to place the label. *Text Label* dialog will open.
3. Write the text in the *Text* field.
4. Select the font by clicking the *Font* button.
5. Enter the *Orientation* of the text (0 degrees equals horizontal position).
6. Select the *Anchor point* for the text.
7. Use *Assign to - Workplace*, if you want the text to stay in the same location regardless of the opened chromatogram (labels stored in the desktop file). Or use *Assign to - Active Signal*, if you want the text to shift as the chromatogram signal moves, zooms in and out (labels stored in the chromatogram file). The text will be displayed only when the respective chromatogram signal is active.
8. Click the *OK* button to accept the settings.



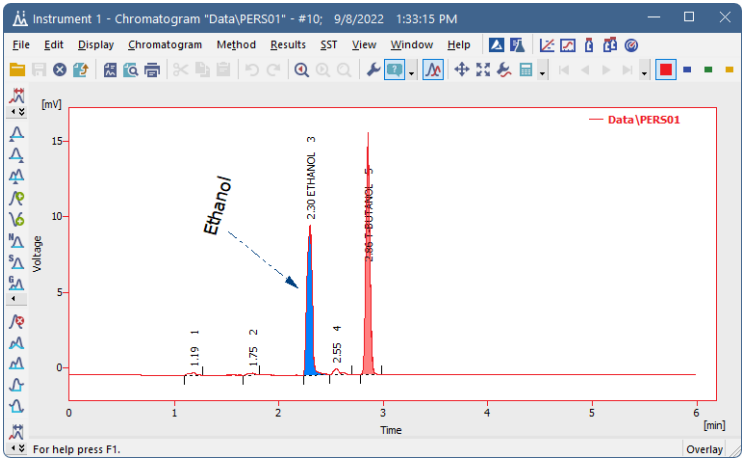
9. Click and drag the text if you wish to move it to a different location.
10. Double-click the text to open *Text Label* dialog to adjust the label settings or to delete it.

Adding line label

1. Right-click in the chromatogram graph to invoke context menu and select *Create Label - Text*.
2. "L" will appear next to the cursor, click and drag to place the line label. *Line Label* dialog will open.
3. Select whether you want to add an arrow tip at the beginning, end or at both ends of the line.
4. Select the color by clicking the *Color* button.
5. Enter the *Line Width*.
6. Select the *Line Style*.
7. Use *Assign to - Workplace*, if you want the text to stay in the same location regardless of the opened chromatogram (labels stored in the desktop file). Or use *Assign to - Active Signal*, if you want the text to shift as the chromatogram signal moves, zooms in and out (labels stored in the chromatogram file). The text will be displayed only when the respective chromatogram signal is active.
8. Click the *OK* button to accept the settings.



9. Click and drag the line if you wish to move it to a different location. Alternatively drag one of the ends to change its position.
10. Double-click the line to open *Line Label* dialog to adjust the label settings or to delete it.



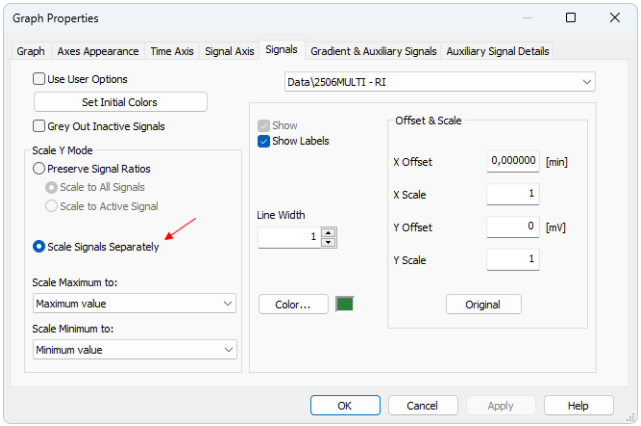
9.6 Working with individual signals of a multisignal chromatogram smoothly

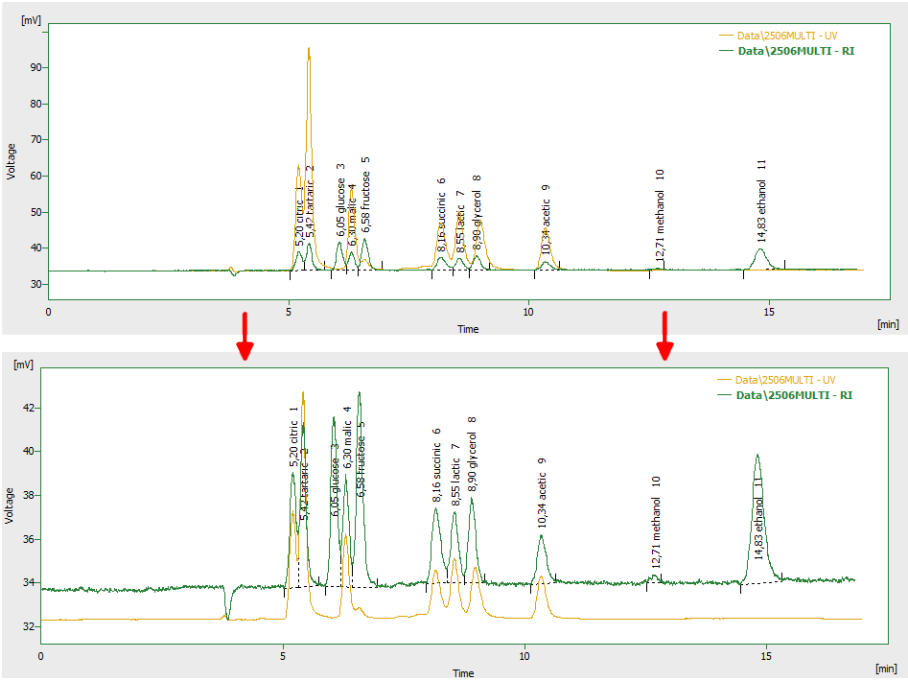
There are some tips on how you can enhance your workflow so that working with multiple signals is more convenient.

9.6.1 Individual scaling of signals

If the signals in the chromatogram have significantly different peak heights, individual scaling can be used to extend both signals over the entire area of the graph.

In the *Graph properties - Signals* tab, select the option *Scale Signals Separately*.

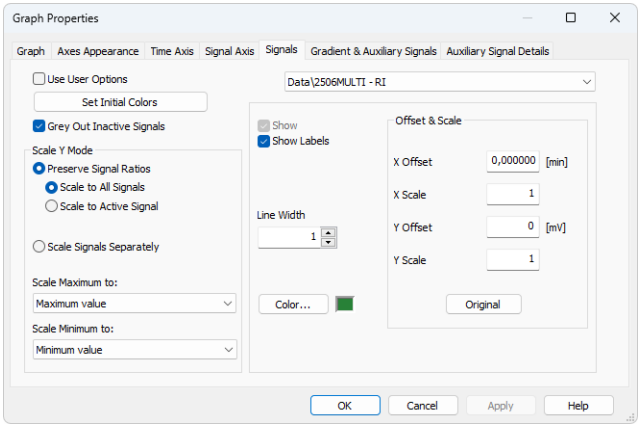


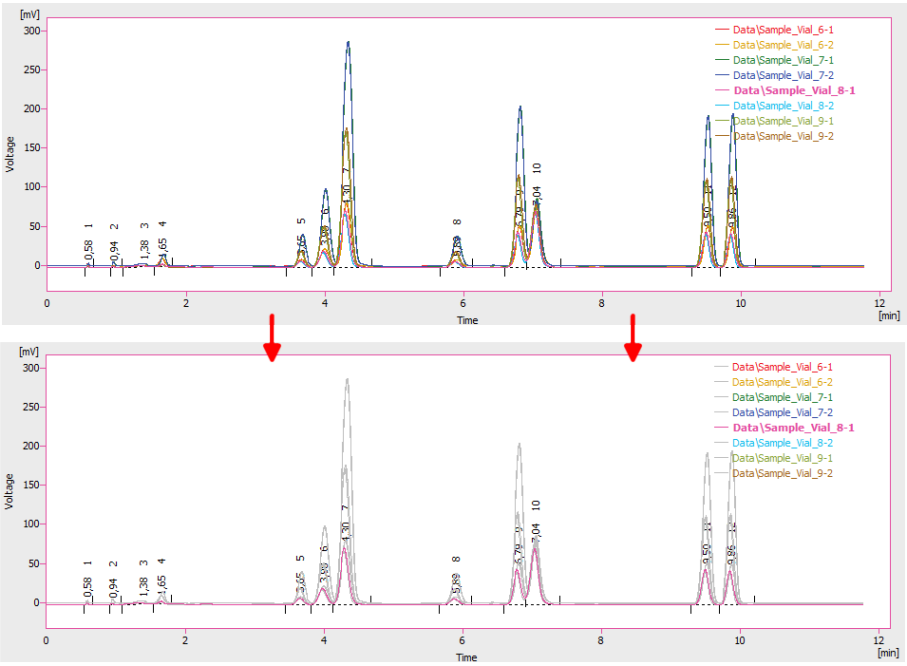


9.6.2 Graying out

To minimize the distraction by the other signals, it is possible to have inactive signals grayed out.

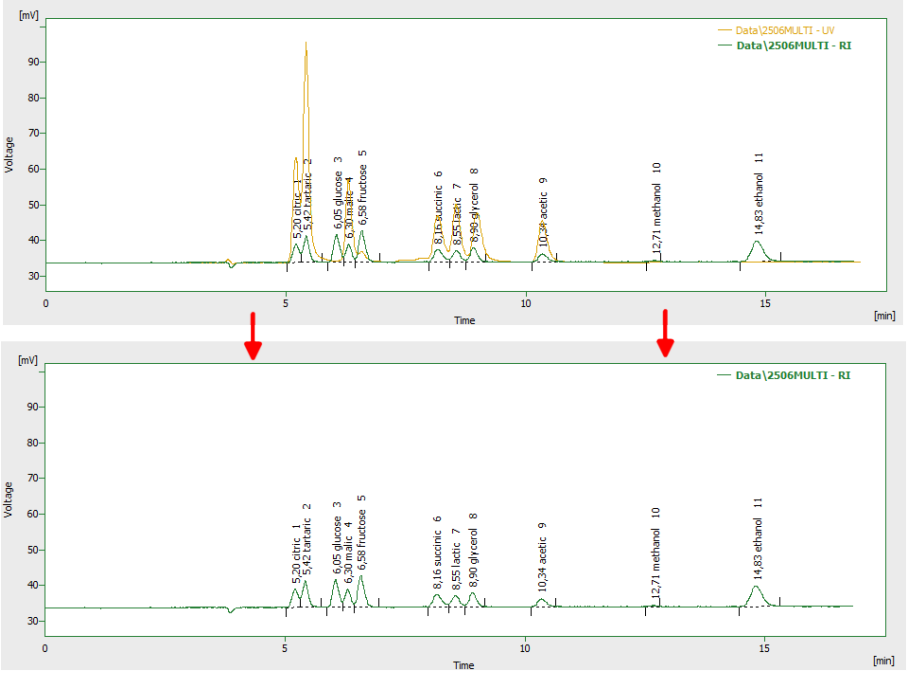
In the *Graph properties - Signals* tab, check the option *Grey Out Inactive Signals*.





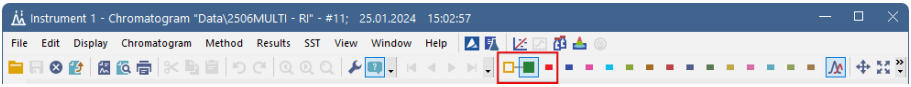
9.6.3 Hiding the signals temporarily

Another option is to hide a signal completely for the session.

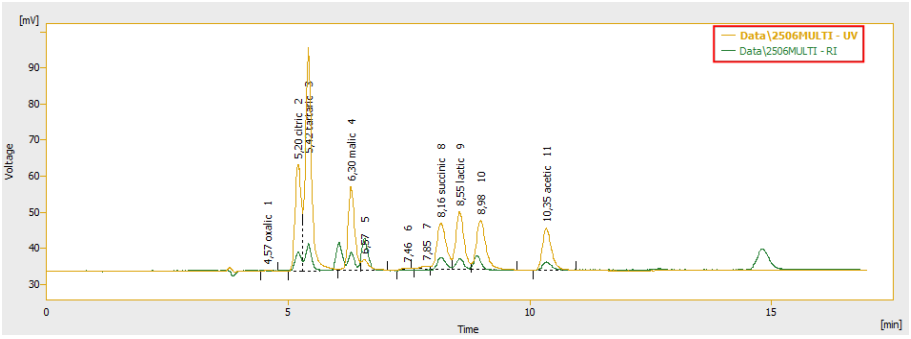


There are more ways how to achieve that:

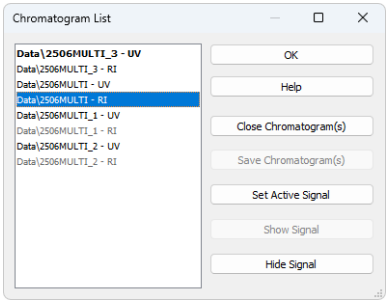
A. Left-click + **CTRL** on the signal color icon in the Toolbar.



B. Double-click + **CTRL** on the name of the signal in the legend.



C. Go to *Chromatogram - Chromatograms...*menu to invoke *Chromatogram List* dialog and select signal(s) to hide.


Chromatogram List
Data\2506MULTI_3 - UV
Data\2506MULTI_3 - RI
Data\2506MULTI - UV
Data\2506MULTI - RI
Data\2506MULTI_1 - UV
Data\2506MULTI_1 - RI
Data\2506MULTI_2 - UV
Data\2506MULTI_2 - RI
OK
Help
Close Chromatogram(s)
Save Chromatogram(s)
Set Active Signal
Show Signal
Hide Signal

10 Calibration

The following chapters contain multiple topics which will guide you through the basic principles of using calibrations in **Clarity** and also introduce you to advanced solutions, for example using the *Bracketing*.

Clarity videos covering calibration-related topics can be found in the Clarity Calibration playlist.

The typical workflow for individuals conducting routine analyses should include:

Preparation of the calibration:

1. Create the calibration. For more details, see the Creating a new calibration topic.
2. Add the number of standard levels you use. For more details, see the Adding a new calibration level topic.
3. If necessary, adjust the calibration according to your needs. For more details, see the Adjusting a calibration topic.

For creating a calibration that will serve as model for calibration cloning, check also the Creating a model calibration for calibration cloning topic.

Linking the calibration to chromatograms:

- It is possible to link the calibration to chromatograms directly. For more details, see the Setting a calibration in a chromatogram topic.
- Or it is possible to link the calibration to a method, so all chromatograms measured using this method will have the specified calibration linked. For more details, see the Setting a calibration in a method topic.

Recalibration:

- In most cases, it is efficient to perform the recalibration automatically from the sequence. For more details, see the Recalibrating automatically using a sequence topic.
  We recommend using calibration cloning on the first recalibration if you want to include only the responses from currently measured sequence in the calibration. For more details, see the Calibrating using clone on first recalibration topic.
- It is also possible to recalibrate from previously measured standards. For more details, see the Recalibrating a calibration topic.

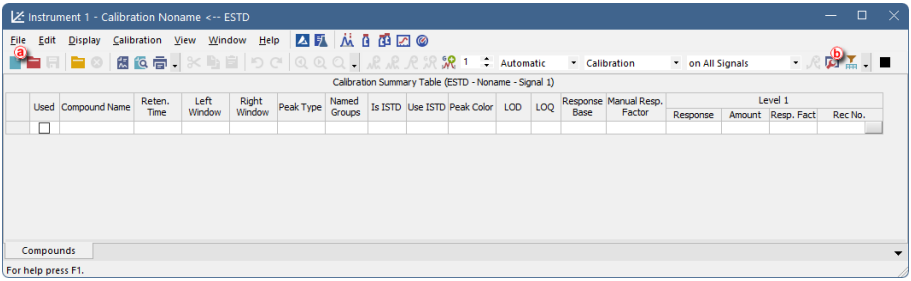
Advanced Topics

Collection of more advanced calibration workflows.

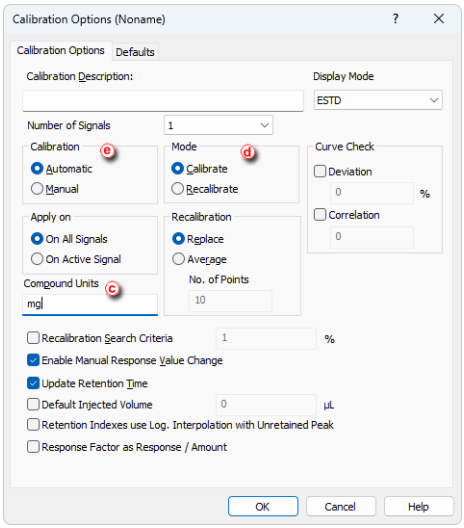
10.1 Creating a new calibration

This chapter covers creating a calibration file. You should have at least one integrated measured standard to be able to fill in the desired peaks into the newly created calibration.

1. Open the Calibration window: choose *Window* - *Calibration* in the *Instrument* window or click

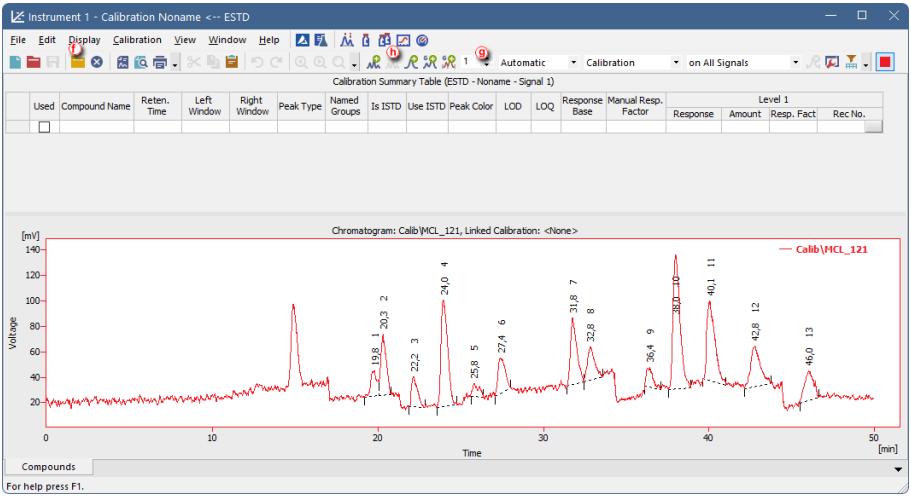


2. Create a new calibration file: select *File - New* or click ⓐ .
3. Open the *Calibration Options* dialog: choose *Calibration - Options…* or click ⓑ .

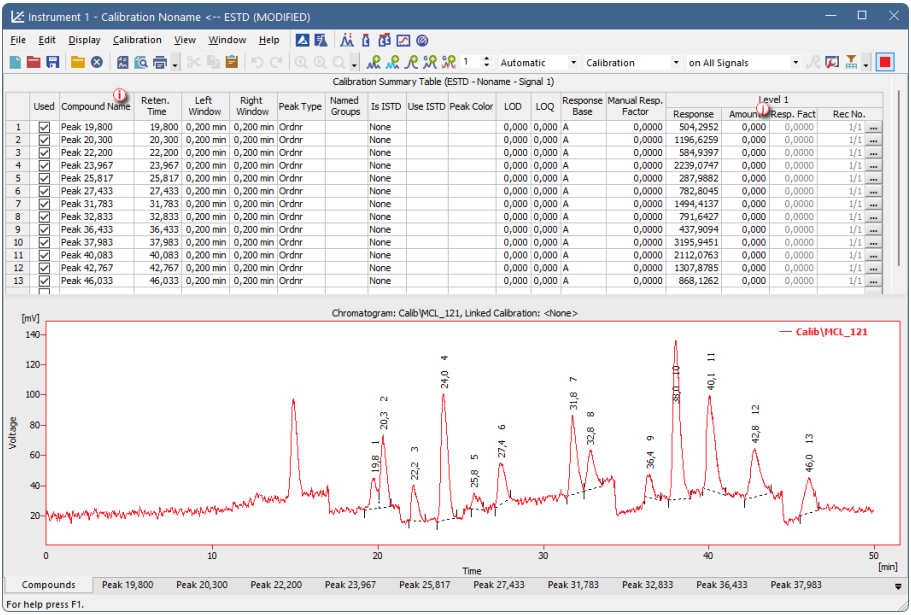


4. Fill in the units in the *Compound Units* section ⓒ to suit your analysis conditions.
5. Set the *Mode* to *Calibrate* ⓓ .
6. Set the *Calibration* option to *Automatic* to add the peaks without modification or *Manual* to modify them one by one ⓔ .
7. Open integrated chromatogram of a standard: choose *File - Open Standard…* or click on ⓕ in the *Calibration* window.
8. Add peaks belonging to the compounds of interest from the chromatogram of the standard to the calibration file.

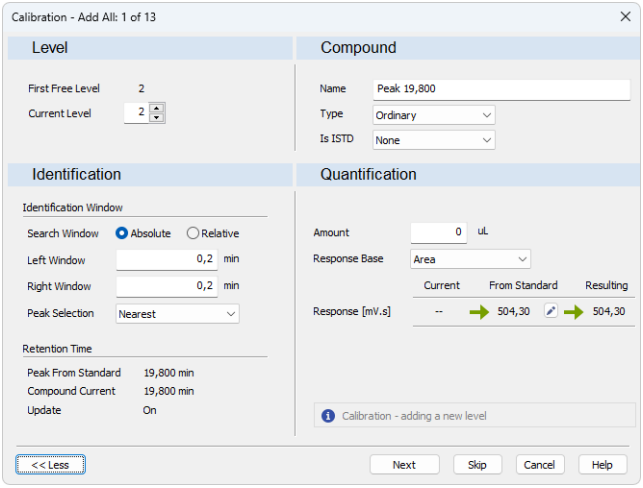
Note: Select *Calibration - Add All* or click on to add all integrated peaks or the Add Peak / Add Group icons to add specific peaks ⓗ. Regardless of the set Current Level ⓖ the peaks will be added to the first free level.



9. If you selected *Automatic* calibration:
   - Name the peaks identified in the *Calibration Summary Table* ⓘ by their retention times by typing the *Compound Name* for each peak. No compound name may be used more than once.
   - Fill in the *Amount* ⓙ for each compound into the *Calibration Summary Table*.



10. If you selected *Manual* calibration: Fill in the Amount, the Compound Name and set any other parameters related to the peak on the *Calibration - Add Peak* window. This window will open once for each one of the peaks processed.

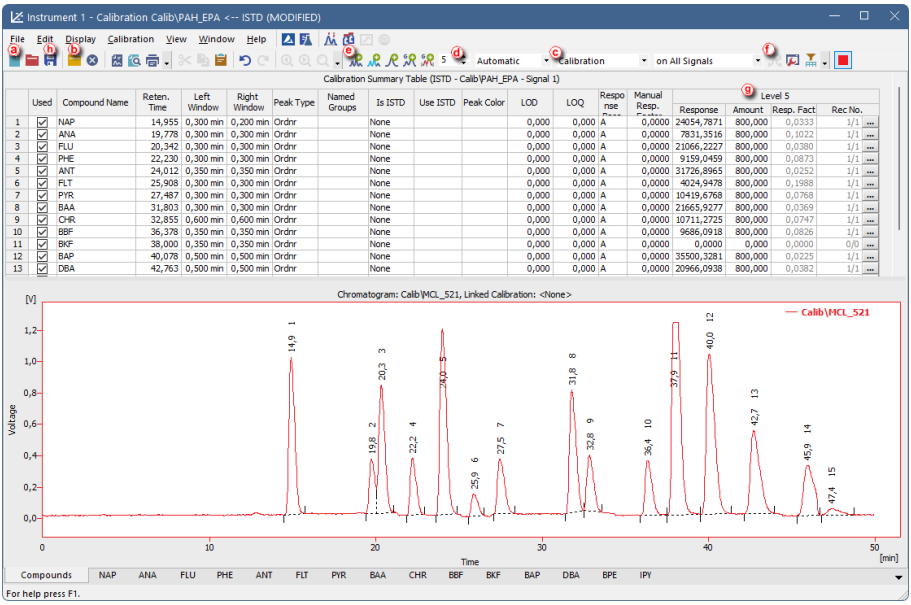


11. Save the calibration file - *File - Save* or click .

10.2 Adding a new calibration level

Here we describe how to add concentration levels to the calibration file to obtain the calibration curve of all compounds. This procedure has to be repeated several times, once for each calibration level to be added.

1. Open the Calibration window: choose *Window - Calibration* on the Instrument window or click icon.



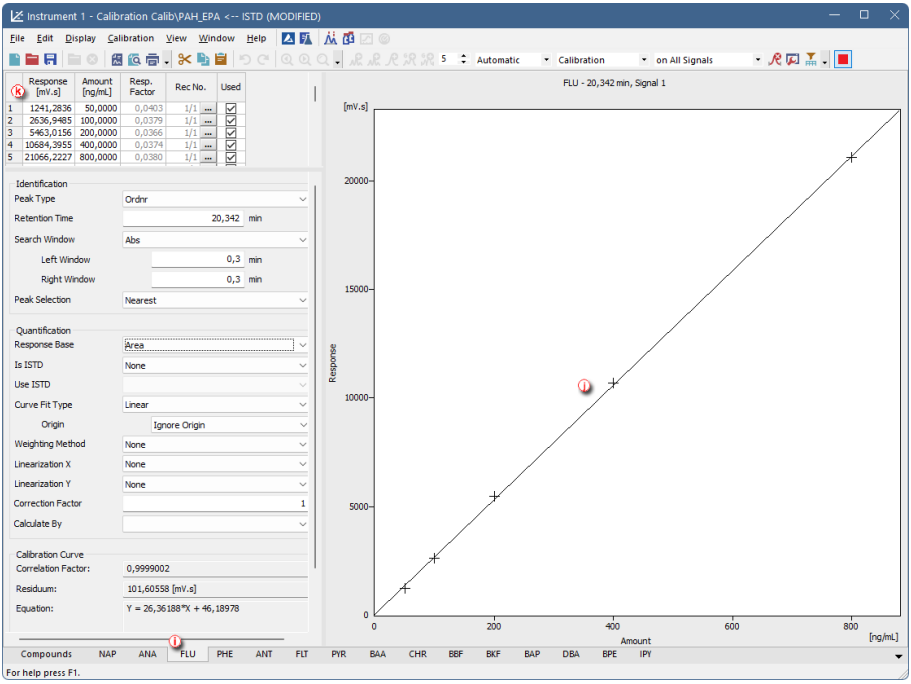
2. Open the calibration file: choose *File - Open…* or click ⓐ .
3. Open calibration standard: select *File - Open Standard…* or click ⓑ .

   Note: Select a measured and qualitatively evaluated chromatogram where all peaks are available, if possible.

4. Check that the *Automatic* option is selected in the first field and the *Calibration* option in the second field of the calibration mode settings ⓒ .
5. The calibration level number is in the *Current Level* field ⓓ set automatically to the first free level.
6. Add all peaks in the chromatogram of the calibration standard to the calibration file: select *Calibration - Add All* or click ⓔ .

Note: In case more peaks than expected emerge in the calibration, the surplus peaks can be deleted by selecting them in the *Calibration Summary Table* and deleting them using *Calibration - Delete Compound* or clicking on ⓕ .

7. Set the amounts of the particular compounds into the *Calibration Summary Table*, into the *Amount* column ⓖ of the respective calibration level.
8. Save the calibration file: choose *File - Save* or click ⓗ
9. Click any tab below ⓘ and you will be able to see the calibration curve ⓙ with all the levels added for one specific compound ⓚ .

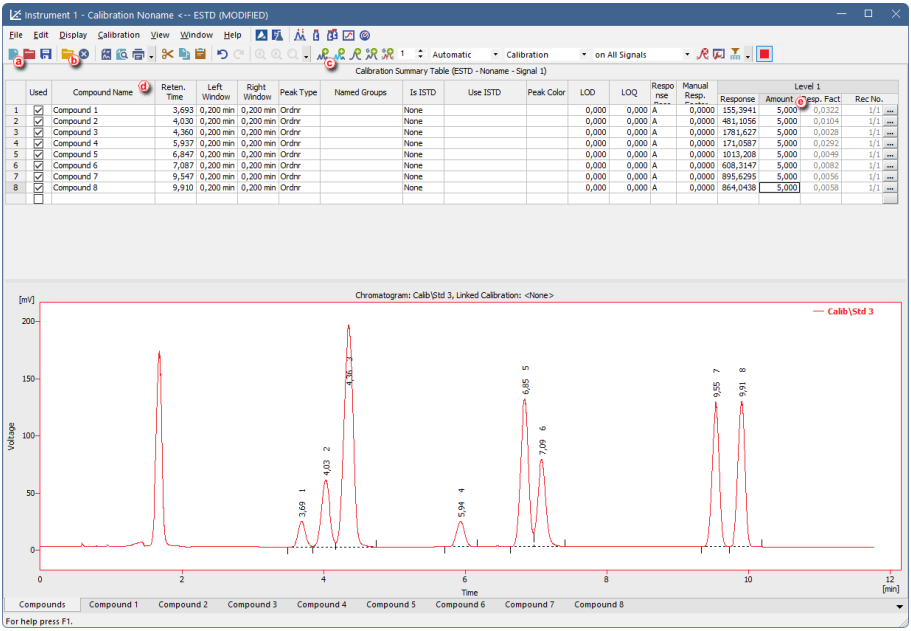


10.3 Creating a model calibration for calibration cloning

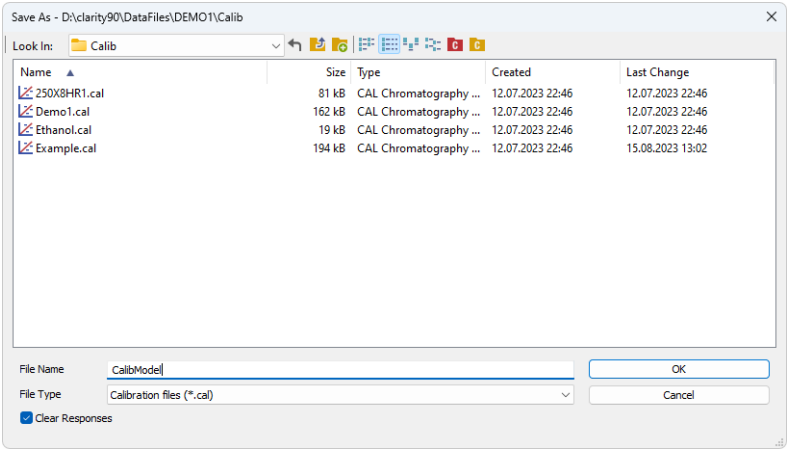
This topic will show you how to prepare model calibration to be used during calibration cloning. If you have calibration already created from the previous measurement skip to step 4.

1. In the *Calibration* window, select *New* ⓐ calibration and *Open* ⓑ typical chromatogram as standard.
2. Use *Add All* ⓒ to add the integrated peaks to calibration.

3. Fill in the *Compound Names* ⓓ and the *Amounts* ⓔ for every level that will be used.



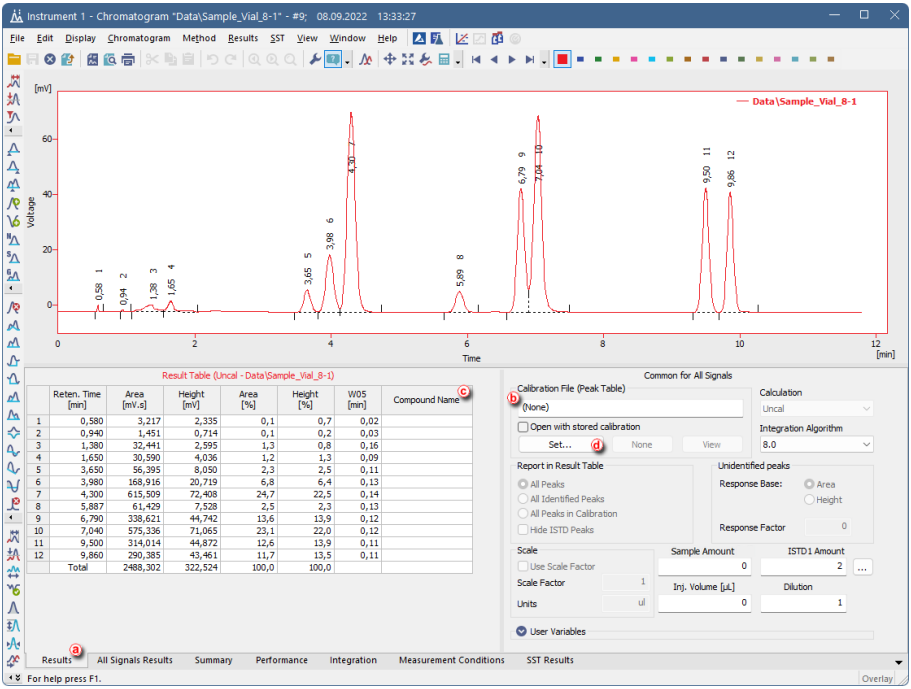
4. Select the *Save As* option. In the *Save As* dialog check the *Clear Responses* checkbox and save the calibration under a new name.



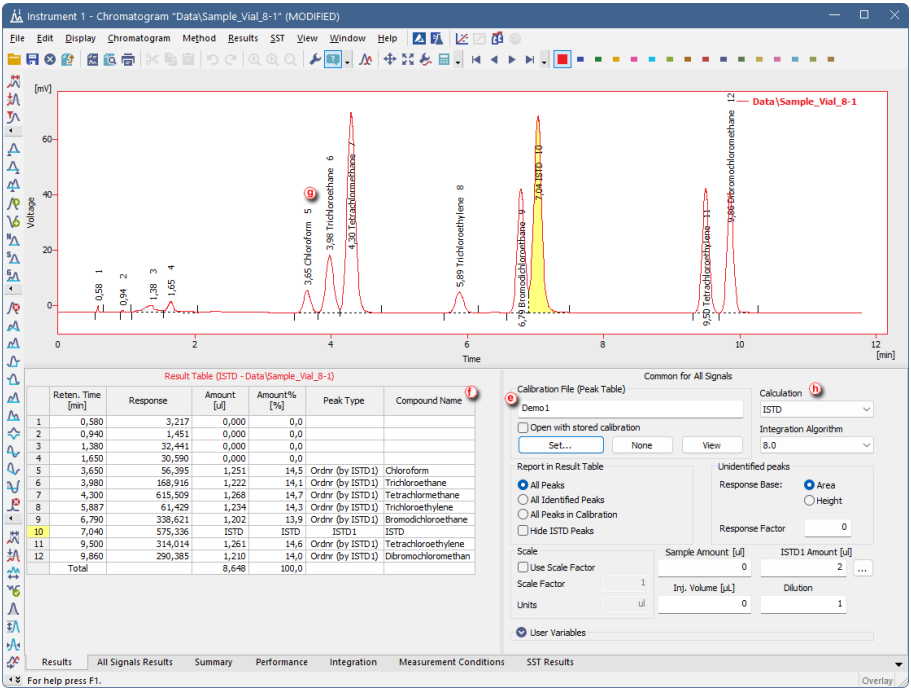
10.4 Setting a calibration in a chromatogram

If the calibration file was not assigned in the method, the measured chromatogram will not have it linked either. Here you will learn how to link a calibration file to a chromatogram.

1. Switch to the *Results tab* ⓐ at the bottom part of the *Chromatogram window*.



2. Check whether the *Calibration File (Peak Table)* field ⓑ is set to *(None)*. If that is the case, then the chromatogram does not have a calibration file linked to it.
3. Also check the *Compound Names* ⓒ in the Result Table section. This column must be empty.
4. To link the calibration file to the Chromatogram, click the *Set…* button ⓓ in the right section of the *Results tab*. You will get a list of all calibrations available in the present project.
    5. Select the correct calibration file from the list and click *OK*. The content of the Chromatogram window will change.

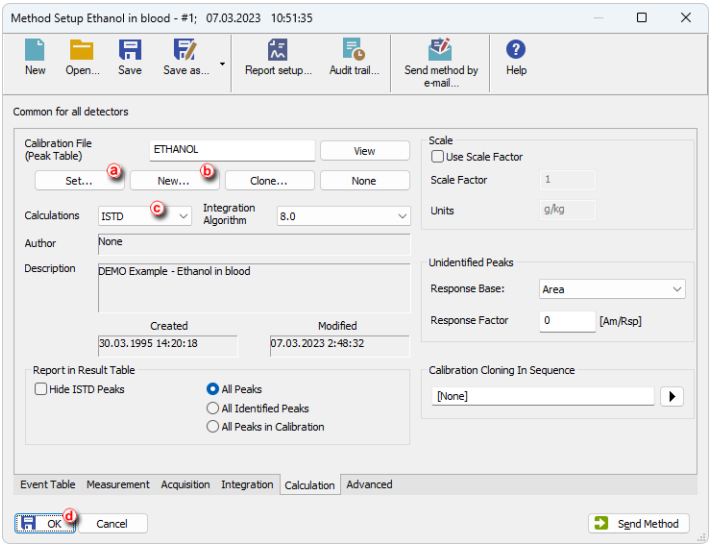


6. Check that the *Calibration File (Peak Table)* field contains the name of the calibration file. ⓔ
7. The *Compound Name* column ⓕ in the *Result Table*, as well as the identified peaks in the graph ⓖ , will now have the names of the identified peaks from the calibration file.
8. Check the *Calculation* field ⓗ to see the type of calculation performed on the chromatogram.
9. Save the chromatogram: select *File - Save* or click .

10.5 Setting a calibration in a method

After the acquisition is performed according to a method, the resulting chromatogram files may be calibrated using a specific calibration. If you need to measure a large number of similar samples, it would be advisable to define a calibration file prior to the acquisition.

1. Open the template method from the Instrument window by using the *Method - Method Setup* command.
2. Go to the *Calculation* tab.

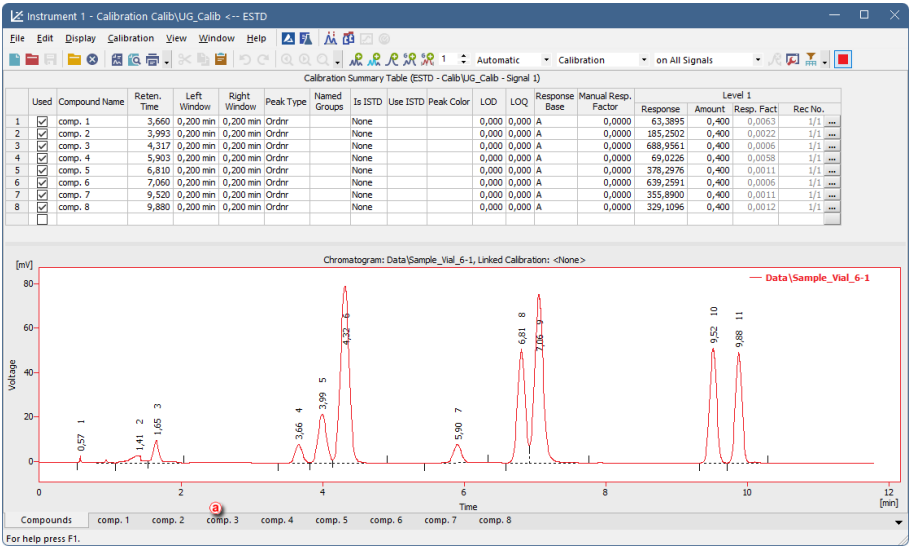


3. Click the *Set…* button ⓐ to select a calibration file for the method, or create a new calibration file by clicking the *New…* button ⓑ .
4. Change the default calibration type in the *Calculations* field ⓒ .
5. Click *OK* ⓓ to save the changes to the opened method.
6. You can modify the calibration file after acquisition. For more info go to *Apply the calibration to a Chromatogram*.

10.6 Adjusting a calibration

Following articles will describe how to perform some of the most common calibration modifications that can improve your calibration. Using this guide you manage to fit your calibration closer to your analytical application.

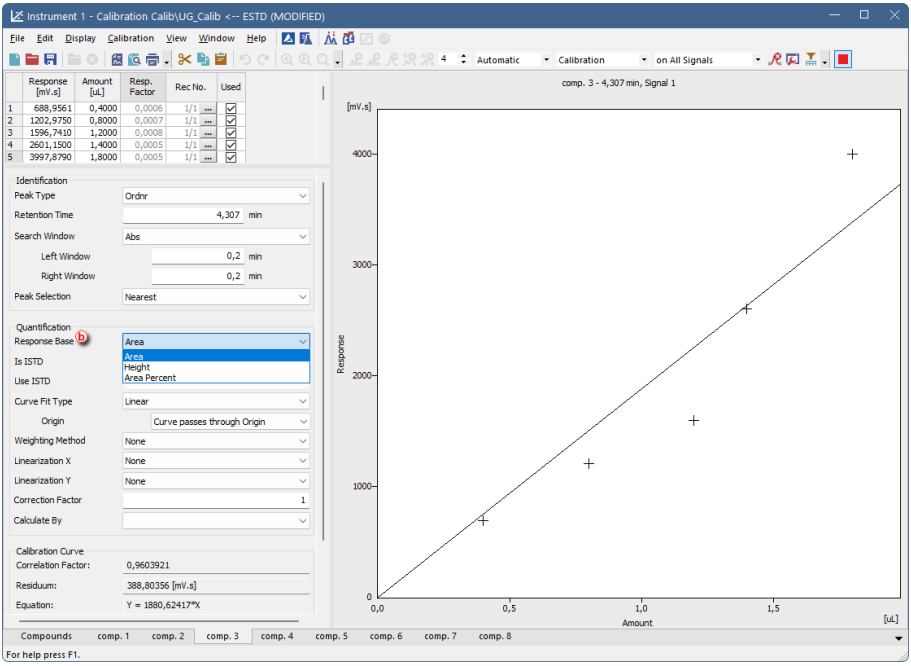
Once you added all chromatograms to your calibration and filled ***Amount*** values for all compounds and all levels, you can start to adjust it. Note that the ***Amount*** values are the values you know, because they originate from the concentration levels of your calibration solutions. Further adjustments of the calibration are available on the corresponding ***Compound Tabs*** at the bottom of the window. In our case, the Comp No. 3 ⓐ is edited.



	Used	Compound Name	Reten. Time	Left Window	Right Window	Peak Type	Named Groups	Is ISTD	Use ISTD	Peak Color	LOD	LOQ	Response Base	Manual Resp. Factor	Level 1 Response	Level 1 Amount	Level 1 Resp. Fact	Level 1 Rec No.
1	☑	comp. 1	3,660	0,200 min	0,200 min	Ordnr		None			0,000	0,000	A	0,0000	63,3895	0,400	0,0063	1/1
2	☑	comp. 2	3,993	0,200 min	0,200 min	Ordnr		None			0,000	0,000	A	0,0000	185,2502	0,400	0,0022	1/1
3	☑	comp. 3	4,317	0,200 min	0,200 min	Ordnr		None			0,000	0,000	A	0,0000	688,9561	0,400	0,0006	1/1
4	☑	comp. 4	5,903	0,200 min	0,200 min	Ordnr		None			0,000	0,000	A	0,0000	69,0226	0,400	0,0058	1/1
5	☑	comp. 5	6,810	0,200 min	0,200 min	Ordnr		None			0,000	0,000	A	0,0000	378,2976	0,400	0,0011	1/1
6	☑	comp. 6	7,060	0,200 min	0,200 min	Ordnr		None			0,000	0,000	A	0,0000	639,2591	0,400	0,0006	1/1
7	☑	comp. 7	9,520	0,200 min	0,200 min	Ordnr		None			0,000	0,000	A	0,0000	355,8900	0,400	0,0011	1/1
8	☑	comp. 8	9,880	0,200 min	0,200 min	Ordnr		None			0,000	0,000	A	0,0000	329,1096	0,400	0,0012	1/1

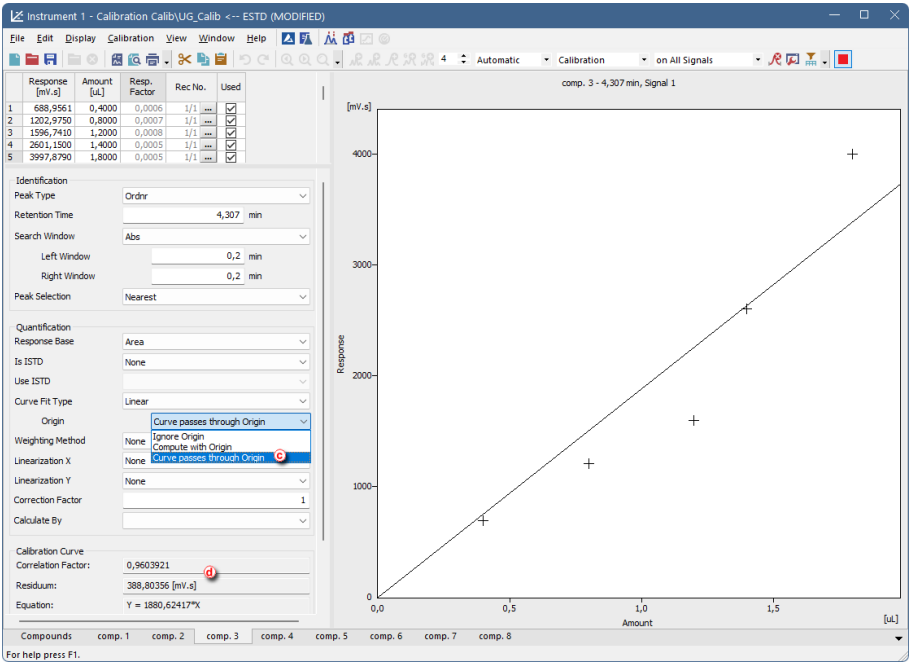
Modifying Response Base

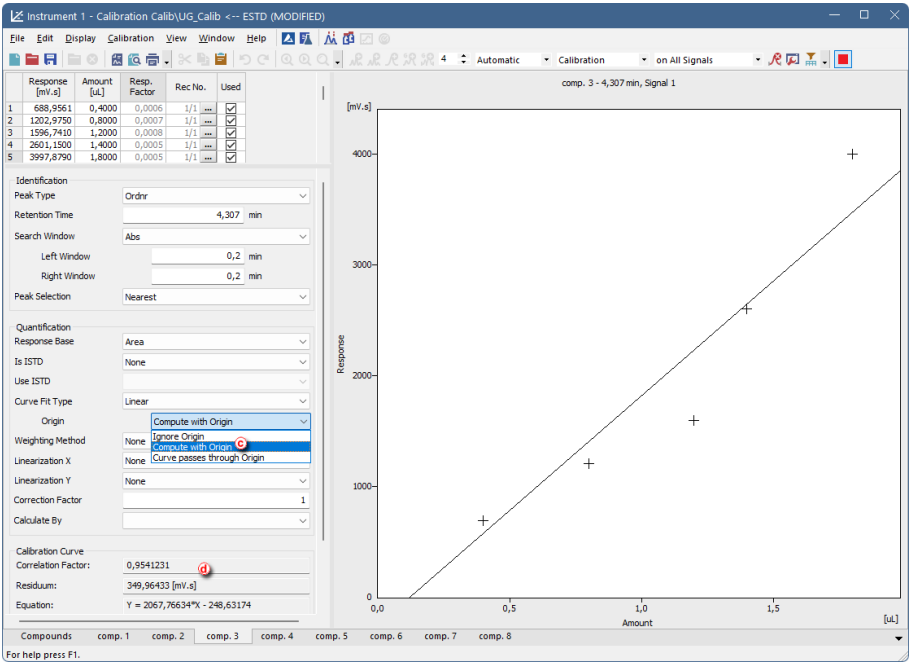
Set the *Response Base* ⓑ to modify whether the calibration curve will be calculated using *Area* or *Height* of the corresponding peak belonging to the specific compound. Changing the *Response Base* can help to create better fitting of the calibration to not well resolved peaks.

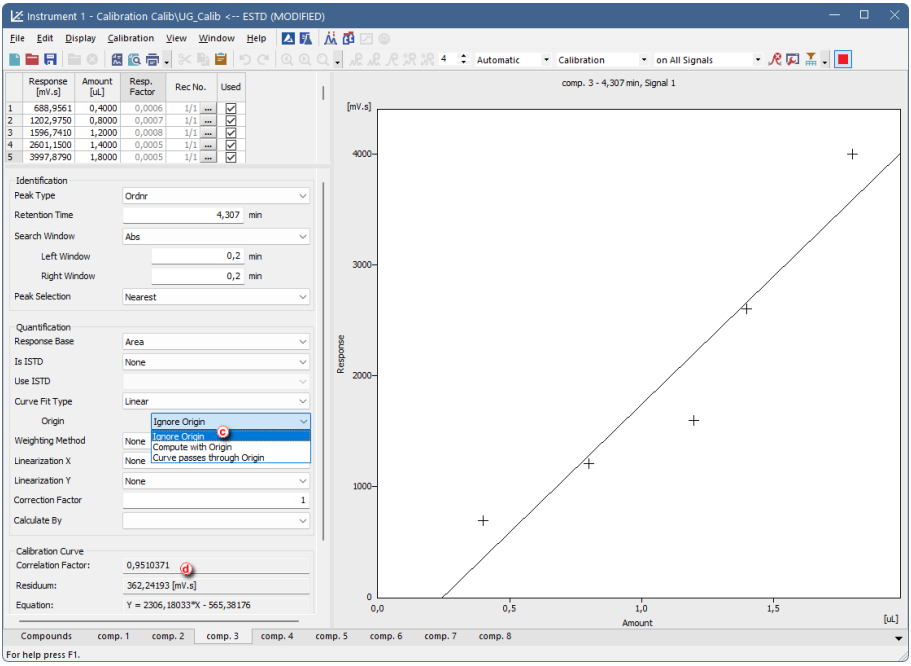


Modifying Origin

Another option how to improve your calibration is setting of *Origin* ⓒ and its incorporation or exclusion in calibration calculations. In **Clarity** there are three available setting options, as described on the following images. There is also demonstrated an effect of the *Origin* setting on calculated *Equation* and *Correlation factor* ⓓ .


Instrument 1 - Calibration Calib\UG_Calib <-- ESTD (MODIFIED)
File Edit Display Calibration View Window Help
Automatic
Calibration
on All Signals
Response [mV.s]
Amount [uL]
Resp. Factor
Rec No.
Used
1 688,9561 0,4000 0,0006 1/1
2 1202,9750 0,8000 0,0007 1/1
3 1596,7410 1,2000 0,0008 1/1
4 2601,1500 1,4000 0,0005 1/1
5 3997,8790 1,8000 0,0005 1/1
Identification
Peak Type Ordnr
Retention Time 4,307 min
Search Window Abs
Left Window 0,2 min
Right Window 0,2 min
Peak Selection Nearest
Quantification
Response Base Area
Is ISTD None
Use ISTD
Curve Fit Type Linear
Origin Curve passes through Origin
Weighting Method None
Ignore Origin
Compute with Origin
Curve passes through Origin
Linearization X None
Linearization Y None
Correction Factor 1
Calculate By
Calibration Curve
Correlation Factor: 0,9603921
Residuum: 388,80356 [mV.s]
Equation: Y = 1880,62417*X
comp. 3 - 4,307 min, Signal 1
[mV.s]
Response
Amount
[uL]
Compounds comp. 1 comp. 2 comp. 3 comp. 4 comp. 5 comp. 6 comp. 7 comp. 8
For help press F1.


Instrument 1 - Calibration Calib\UG_Calib <-- ESTD (MODIFIED)
File Edit Display Calibration View Window Help
Automatic
Calibration
on All Signals
Response [mV.s]
Amount [uL]
Resp. Factor
Rec No.
Used
1 688,9561 0,4000 0,0006 1/1
2 1202,9750 0,8000 0,0007 1/1
3 1596,7410 1,2000 0,0008 1/1
4 2601,1500 1,4000 0,0005 1/1
5 3997,8790 1,8000 0,0005 1/1
Identification
Peak Type Ordnr
Retention Time 4,307 min
Search Window Abs
Left Window 0,2 min
Right Window 0,2 min
Peak Selection Nearest
Quantification
Response Base Area
Is ISTD None
Use ISTD
Curve Fit Type Linear
Origin Compute with Origin
Ignore Origin
Compute with Origin
Curve passes through Origin
Weighting Method None
Linearization X None
Linearization Y None
Correction Factor 1
Calculate By
Calibration Curve
Correlation Factor: 0,9541231
Residuum: 349,96433 [mV.s]
Equation: Y = 2067,76634*X - 248,63174
comp. 3 - 4,307 min, Signal 1
[mV.s]
Response
Amount
[uL]
Compounds comp. 1 comp. 2 comp. 3 comp. 4 comp. 5 comp. 6 comp. 7 comp. 8
For help press F1.



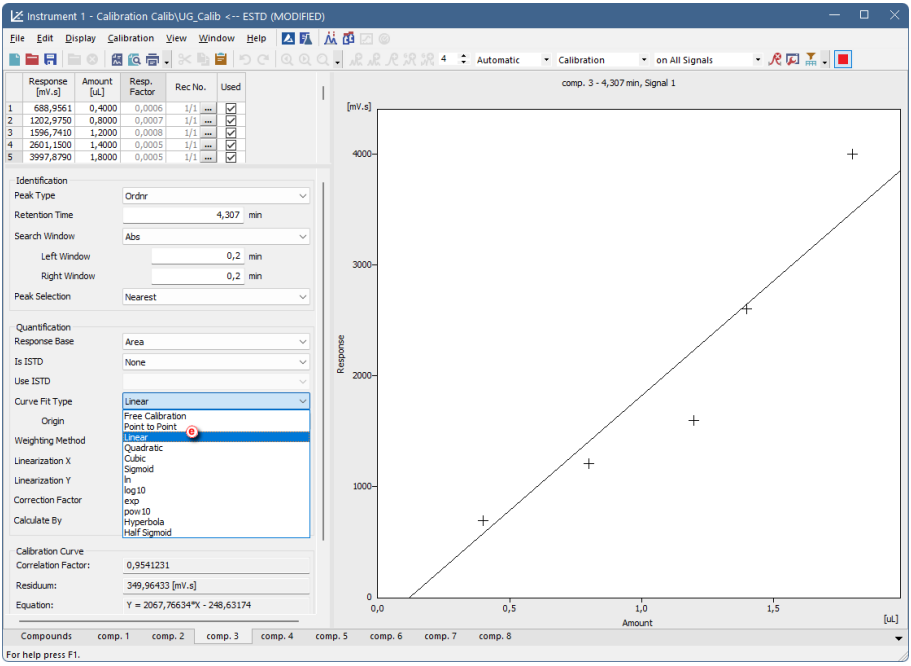
As you can see from the *Correlation factor* ⓓ values, changing the *Origin* setting from the *Curve Passes through Origin* to *Compute with Origin* improved the curve fit. However, the option *Ignore Origin* has proved to be the best match for the used detector.

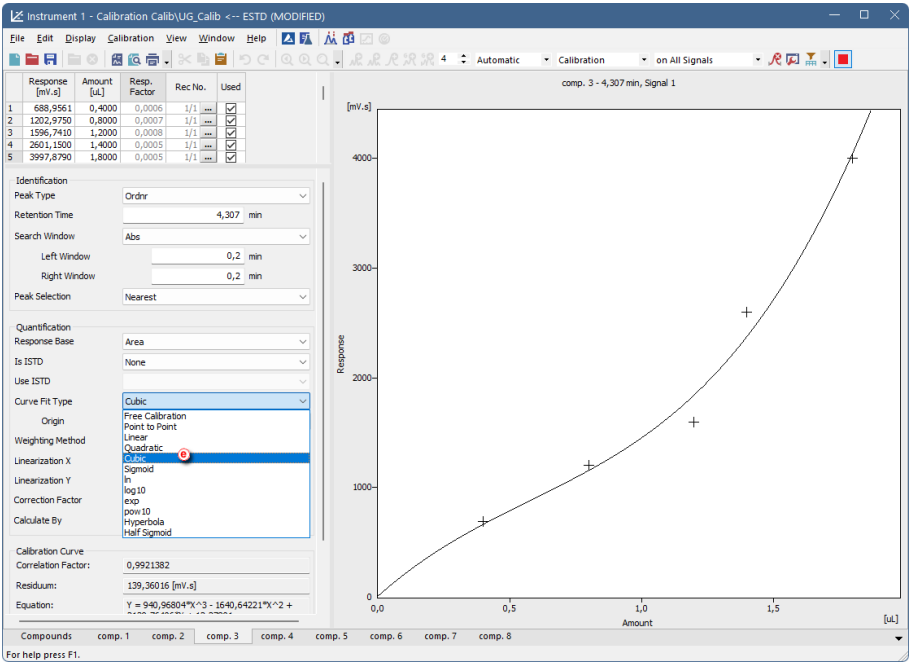
Modifying Curve Fit Type

Following images demonstrate how to modify *Curve Fit Type* ⓔ from *Linear* to *Cubic*. *Cubic Curve Fit Type* is used as an example of non-linear *Curve Fit Types*.

- Linear calibration curve is commonly used for detectors with linear response, such as Flame Ionization Detector (FID) or Refractive Index Detector (RID).
- Non-linear calibration curve is typical for detectors such as Electron Capture Detector (ECD) or Evaporative Light Scattering Detector (ELSD).

When changing *Curve Fit Type* ⓔ pay also attention to the values of the calculated *Equation* and *Correlation Factor*. Increasing value of the *Correlation Factor* indicates better selected *Curve Fit Type* for the measured data.

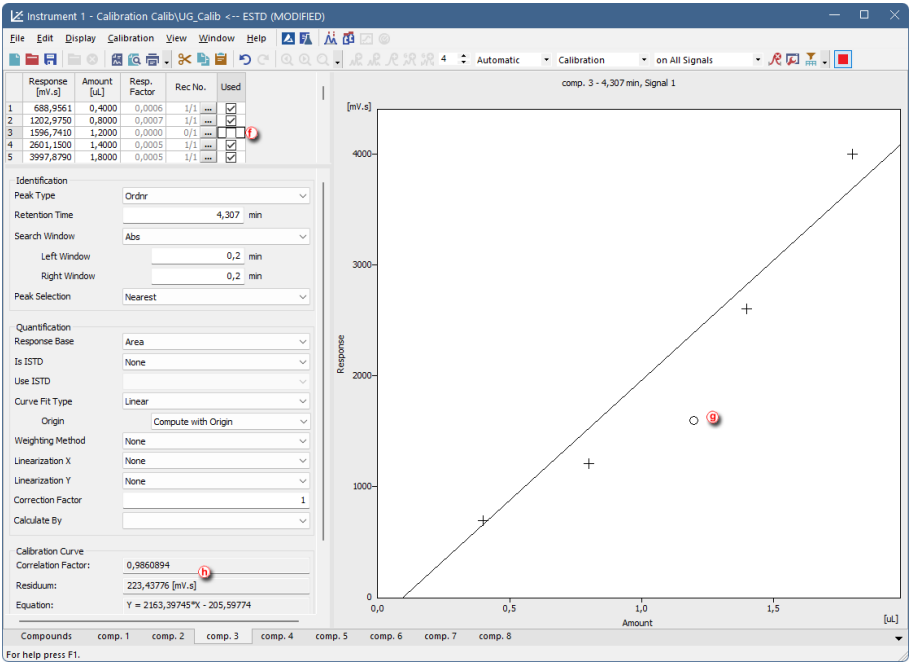

Instrument 1 - Calibration Calib\UG_Calib <-- ESTD (MODIFIED)
File Edit Display Calibration View Window Help
Automatic
Calibration
on All Signals
Response [mV.s]
Amount [uL]
Resp. Factor
Rec No.
Used
1 688,9561 0,4000 0,0006 1/1
2 1202,9750 0,8000 0,0007 1/1
3 1596,7410 1,2000 0,0008 1/1
4 2601,1500 1,4000 0,0005 1/1
5 3997,8790 1,8000 0,0005 1/1
Identification
Peak Type Ordnr
Retention Time 4,307 min
Search Window Abs
Left Window 0,2 min
Right Window 0,2 min
Peak Selection Nearest
Quantification
Response Base Area
Is ISTD None
Use ISTD
Curve Fit Type Linear
Origin
Weighting Method
Linearization X
Linearization Y
Correction Factor
Calculate By
Free Calibration
Point to Point
Linear
Quadratic
Cubic
Sigmoid
ln
log10
exp
pow10
Hyperbola
Half Sigmoid
Calibration Curve
Correlation Factor: 0,9541231
Residuum: 349,96433 [mV.s]
Equation: Y = 2067,76634*X - 248,63174
comp. 3 - 4,307 min, Signal 1
[mV.s]
Response
Amount
[uL]
Compounds comp. 1 comp. 2 comp. 3 comp. 4 comp. 5 comp. 6 comp. 7 comp. 8
For help press F1.



As you can see, changing the *Curve Fit Type* from *Linear* to *Cubic* increased the *Correlation Factor* from 0.954 to 0.992.

Excluding of Measured Point from Calibration

Clarity also allows excluding any point from calibration. This is helpful in case that the specific measurement went wrong. Following images describe how to do that. Please keep in mind that the excluded point isn't deleted, the point is still part of the calibration, however, it is omitted from calculation of calibration curve. To exclude the selected measurement point from the calibration simply uncheck that measurement in the *Used* ⓕ column. The excluded point in the graph of calibration curve will be changed from cross to empty circle ⓖ and calibration curve *Equation* and *Correlation Factor* ⓗ will be recalculated.

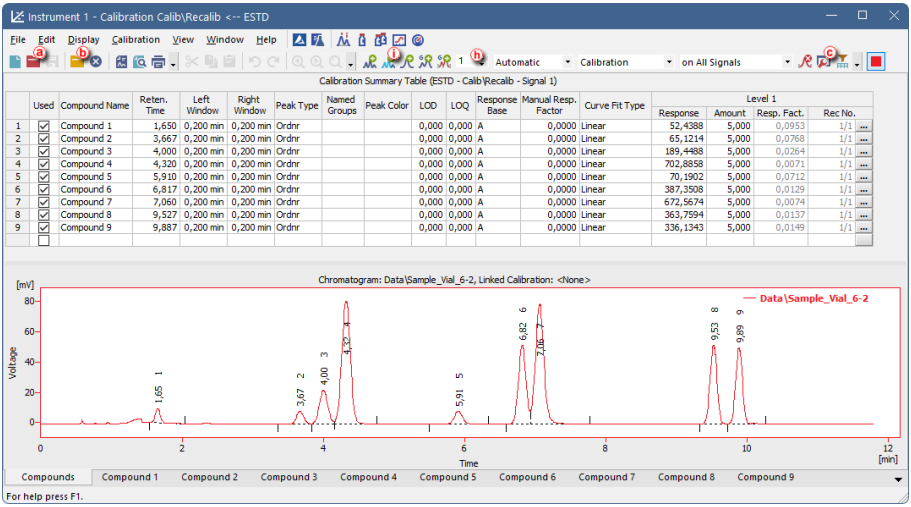


As you can see, excluding the incorrectly measured calibration point resulted in more accurate calibration.

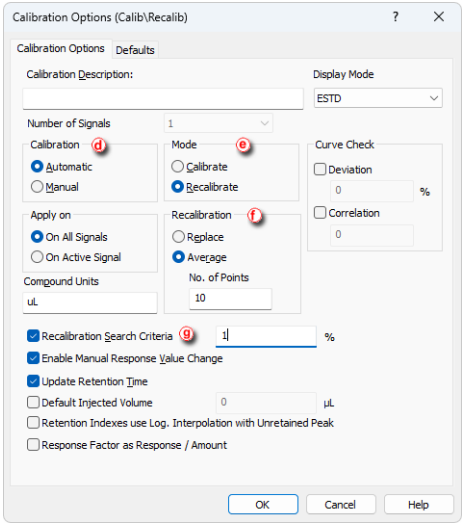
10.7 Recalibrating a calibration

You can modify an existing calibration by reloading peaks within one specific level using the option *Recalibrate*.

1. Open the Calibration window: choose *Window - Calibration* on the *Instrument* window or click .

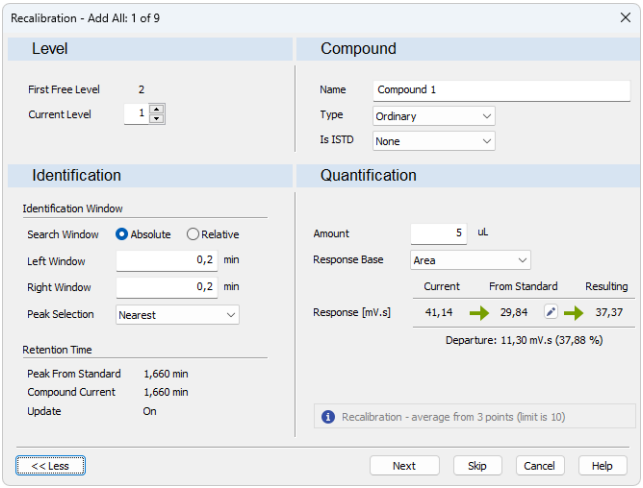


2. Open the calibration file: choose *File - Open…* or click ⓐ .
3. Open the calibration standard with which you want to recalibrate: select *File - Open Standard…* or click ⓑ .
4. Open the *Calibration Options* dialog: choose *Calibration - Options…* or click ⓒ .



5. Set the *Calibration* option to *Automatic* to add the peaks without modification or to *Manual* to modify them one by one ⓓ .

6. Set the *Mode* to *Recalibration* ⓔ .
7. Select how and whether the new values will be added in the *Calibration Options* dialog.
    - Choose *Replace* or *Average* option to decide what to do with new response values ⓕ .
    - *Recalibration Search Criteria* defines how much the original and new values can differ for the recalibration to be performed ⓖ .
8. Select the *Level* you wish to recalibrate ⓗ .
9. Add peaks to be recalibrated from the calibration standard to the calibration file on the *Calibration* window using *Calibration - Add Existing* or clicking on ⓘ .
10. If you selected *Manual* calibration:
    - Fill in any parameters related to the peak in the *Calibration - Add All* window. This window will open once for each one of the peaks processed.

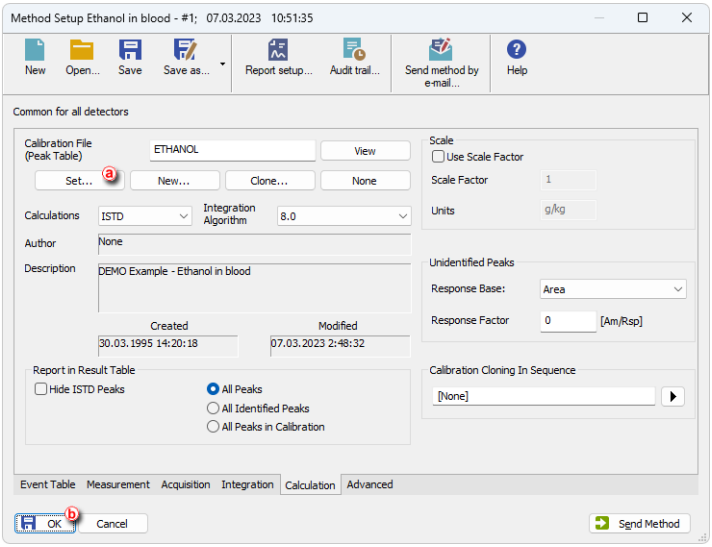


11. Save the calibration file: choose *File - Save* or click on .

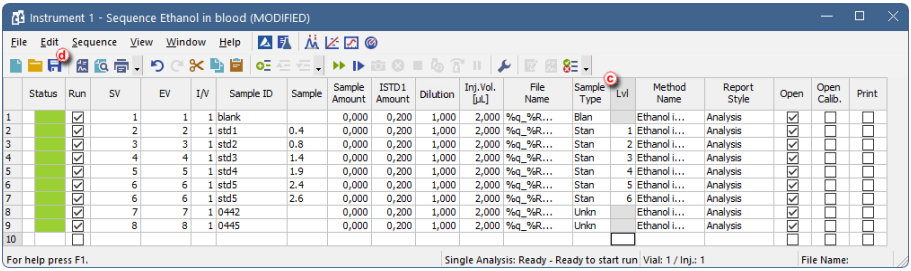
10.8 Recalibrating automatically using a sequence

Here we describe how to add more data to a calibration point from more than one calibration standard chromatogram using a sequence.

1. Open the method file: use *File - Open Method…* on the Instrument window or click in the *Method Setup* dialog.
2. Go to the *Calculation* tab.



3. Connect the calibration file to the method by using the *Set…* ⓐ button.
4. Save the method file - click *OK* ⓑ or select *File - Save Method* or click .
5. Open the Sequence window: select *Analysis - Sequence* or click in the *Instrument* window.



6. Fill in the Sequence Table as described in the section ***Run a sequence***.
7. For the calibration standards, fill in the *Sample Type* and *Lvl* columns ⓒ in the *Sequence Table*.

More Info:

The *Sample Type* column for the calibration standard should be set to the *Standard* value, the *Lvl* column for each standard must have a value between *1* and *20*. For a blank sample, select *Blank* in the *Sample Type* column.

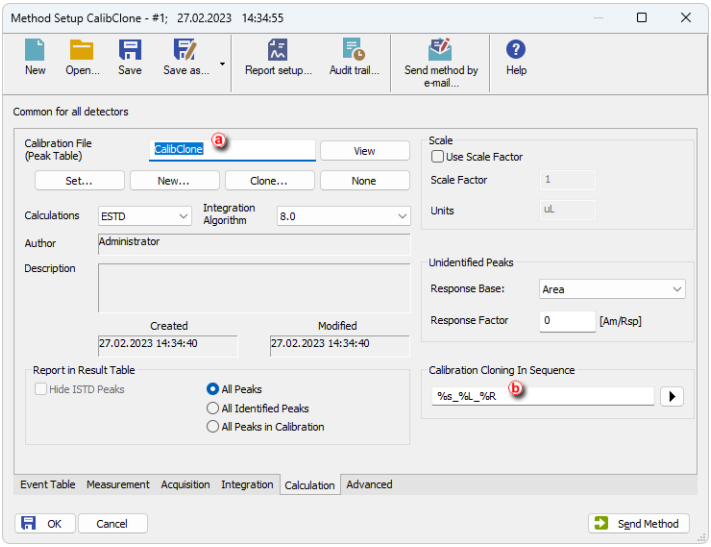
8. Save the sequence file: select *File - Save* or click . ⓓ

The file is now prepared so that the calibration standards measured according to their sequence rows will automatically recalibrate the calibration file.

10.9 Calibrating using clone on first recalibration

Option *Clone on first recalibration* sets the sequence and calibration to the Safe Calibration Usage mode. This option will create a clone (copy) of calibration defined in the method upon completing the first row of the sequence. Cloned calibration is attached to each new chromatogram produced by the given sequence.

1. Open the *Method Setup* dialog - Calculation tab. Select *Method - Calculation* from the *Instrument* window.



2. Click on *Set...* button and select a calibration file ⓐ to be used during cloning at first recalibration.

   Note: This calibration will remain unchanged as newly created clone of the calibration will be used with new responses.

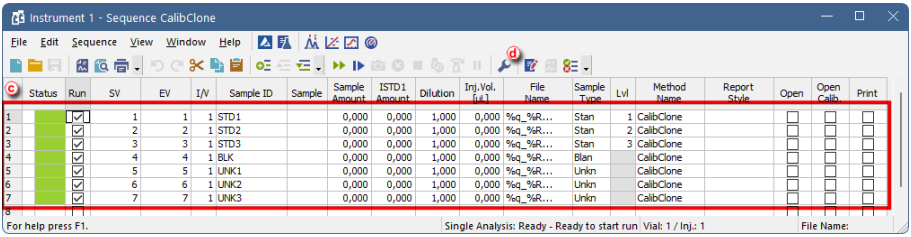
3. Create a custom name for the calibration files in *Calibration Cloning in Sequence* ⓑ as explained in ***Creating customized file names automatically***.

   Note: The name of the final calibration file will match just the content of this field - if you wish to include the name of the template calibration, include the name in this field again (e.g. "test - %s %L %R").

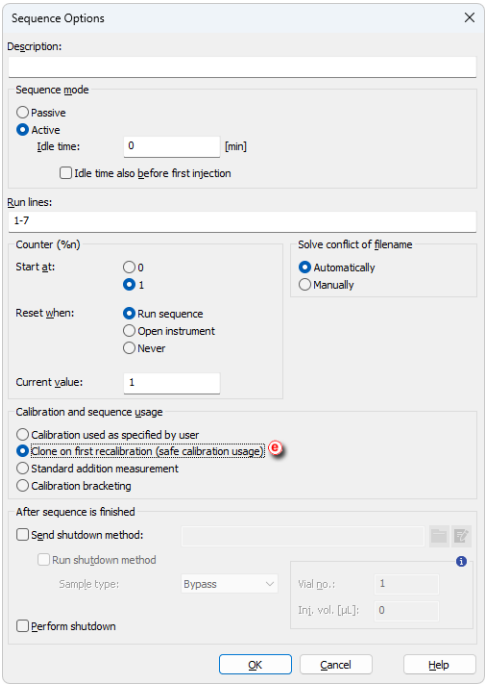
4. Follow the steps in ***Creating and running a sequence*** to create your sequence based on the example below.

More Info:

- Set the row/s for the standard/s at the beginning. ⓒ
- Add a row for a blank, if you wish to.
- Set the row/s for the unknown samples.



5. Click to open the *Sequence Options* Dialog ⓓ .
6. Select *Clone on first recalibration* ⓔ and click *OK*.



7. Run the sequence as explained in ***Creating and running a sequence***.

Note: The measured sequence can be reprocessed using Batch. For more info see the topic Reprocessing whole sequence while using calibration cloning.

10.10 Calibration - Advanced topics

This chapter contains collection of more advanced topics covering calibration usage in Clarity.

10.10.1 Creating a multisignal calibration

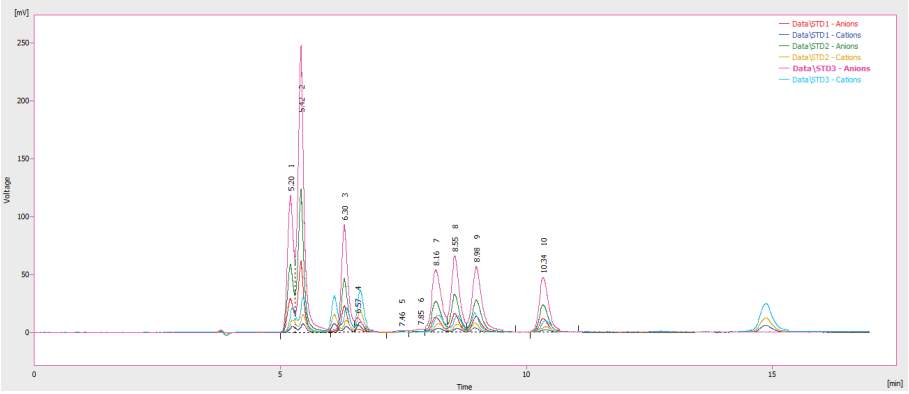
This topic describes how to construct a multisignal calibration in Clarity. Below is an example of creating and constructing a three (concentration) level calibration which provides calculation parameters for calculating results in two- signal chromatograms. This procedure should be utilized when different compounds are detected on each signal. In case all signals detect the same compounds there is no need to use *On Active Signal* option, unless you don't want to quantify all of the compounds on some signals.

Note: For cases there is need to create and construct more than a two-signal calibration, the applied approach remains the same. It varies from the below procedure slightly. These aspects are reflected in the respective steps of this topic.

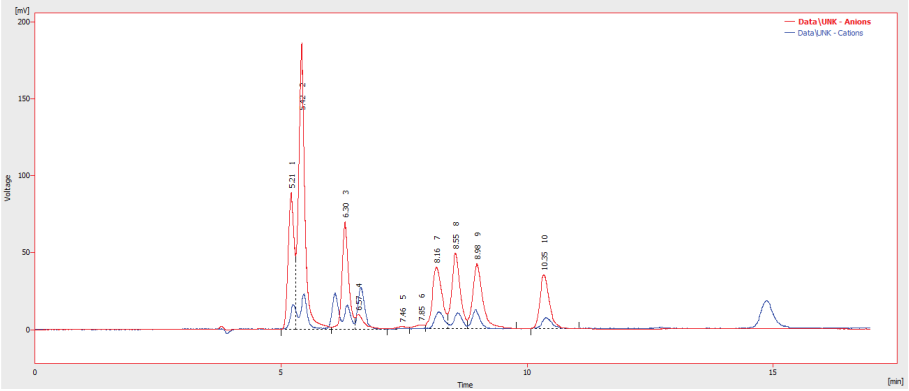
This guide is based on two-signal chromatograms of standards with simulated data (for demonstration purposes it can be said that first signal detects anions and second detects cations) on three concentration levels (5 000 ppm, 10 000 ppm and 20 000 ppm) and one sample chromatogram. All chromatograms used in this guide have been integrated in manner to fit the demonstration purpose.

Prerequisites:

- Integrated chromatograms of standards.

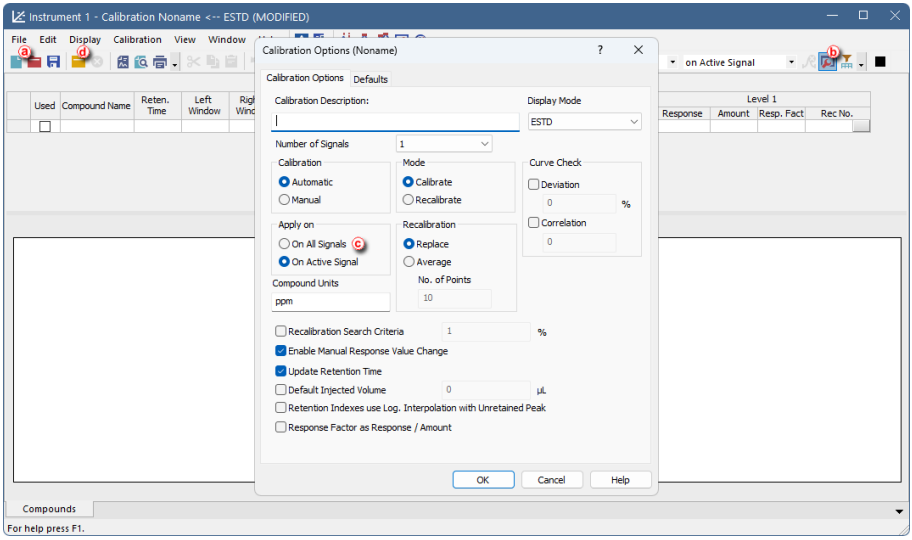


- Integrated chromatogram of sample.



1. Open the Calibration window: select *Window - Calibration* in the *Instrument* window or click .
2. Create a new calibration file: select *File - New* or click ⓐ .
3. Open the Calibration Options dialog: select *Calibration - Options…* or click ⓑ .
4. Set section *Apply on* to option *On Active Signal* field ⓒ .

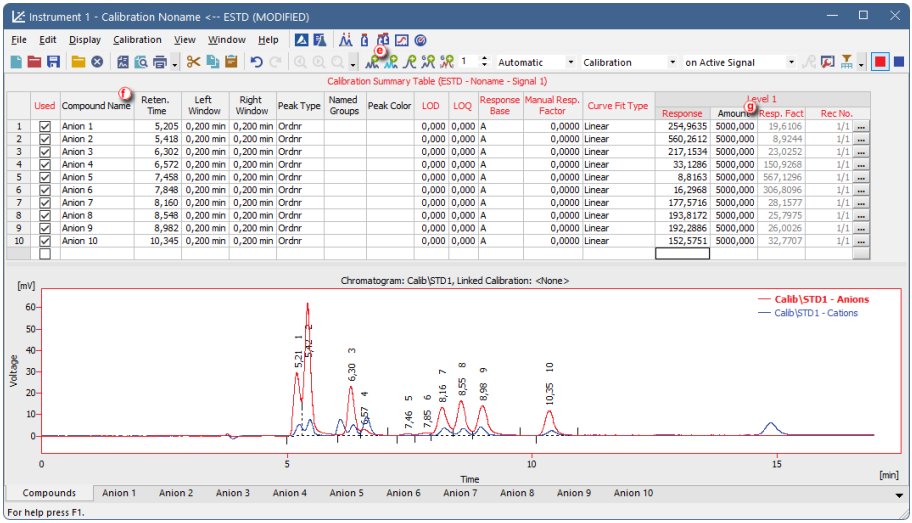
Note: As mentioned in the beginning. If all peaks in the standard chromatogram represent the same compound across all signals it is viable to change the option to *On All Signals*. In such case there is no difference in working with multisignal and single signal calibration.



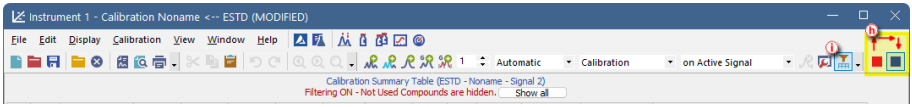
5. Open calibration standard: select *File - Open Standard…* or click ⓓ to open measured and integrated chromatogram with the lowest concentration level where all peaks are available.
6. Make sure the upper toolbar displays *on Active Signal*. It is also recommended to make sure you are currently on the first signal as well (focused red square in right part of the upper toolbar).
7. Fill the *Calibration Summary Table* with peaks from the currently selected signal in chromatogram using the *Add All* icon ⓔ .

   Note: If only some peaks should evaluated it can be done by using *Add Peak* on peaks that need to be included in calibration.

8. Rename automatically pre-filled names of peaks ⓕ .
9. Enter values for given standard into the *Amount* column ⓖ .

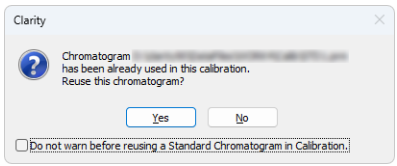


10. Switch to the second signal in chromatogram to make it active ⓗ .
11. Optional: Switch the table filter on using *Filter Not Used Compounds* icon ⓘ . With this option enabled, rows with not *Used* compounds on given signal are hidden, which makes it easier to navigate *Calibration Summary Table*.



12. Fill the *Calibration Summary Table* with peaks from the currently selected (second) signal in chromatogram using *Add All* icon. Dialog will be invoked after clicking *Add All* icon questioning if an already used chromatogram should be reused for this calibration. It is necessary to confirm the reuse by clicking *Yes* button.

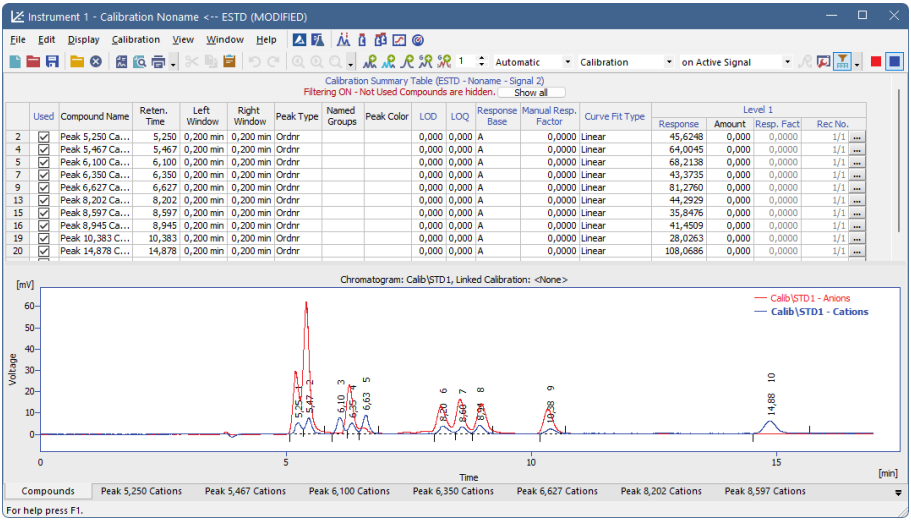
Note: In case of constructing calibration with more than two signals, steps 12 and 14 have to repeated as many times as necessary in order to fill in peaks from all signals to *Calibration Summary Table*.



Note:

This dialog will be invoked multiple times based on number of signals in calibration for calibration with more than two signals. It is possible to switch off invoking of the dialog using the checkbox in the bottom of the dialog.

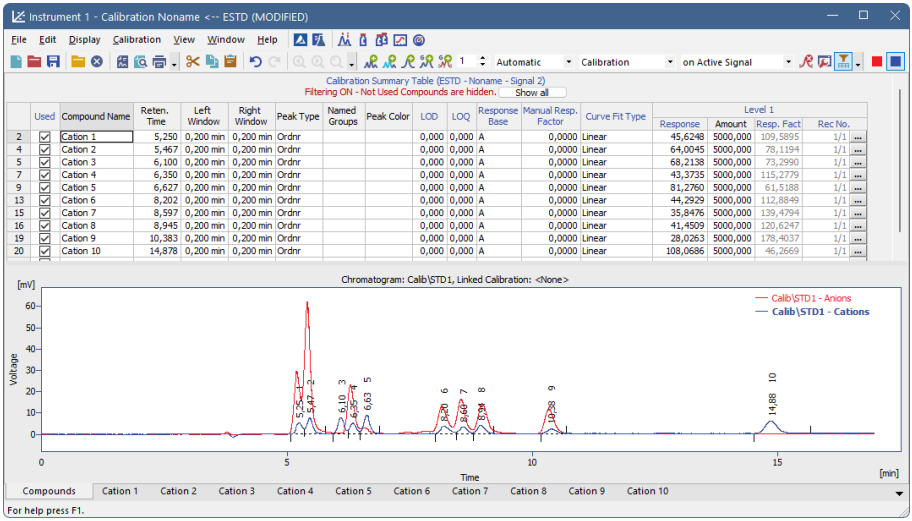
Note: Which signal of chromatogram is active and is being worked with is given by the *Calibration Summary Table* title's color and displayed number of currently active signal.



	Used	Compound Name	Reten. Time	Left Window	Right Window	Peak Type	Named Groups	Peak Color	LOD	LOQ	Response Base	Manual Resp. Factor	Curve Fit Type	Level 1 Response	Level 1 Amount	Level 1 Resp. Fact	Level 1 Rec No.
2	☑	Peak 5,250 Ca…	5,250	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	45,6248	0,000	0,0000	1/1
4	☑	Peak 5,467 Ca…	5,467	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	64,0045	0,000	0,0000	1/1
5	☑	Peak 6,100 Ca…	6,100	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	68,2138	0,000	0,0000	1/1
7	☑	Peak 6,350 Ca…	6,350	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	43,3735	0,000	0,0000	1/1
9	☑	Peak 6,627 Ca…	6,627	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	81,2760	0,000	0,0000	1/1
13	☑	Peak 8,202 Ca…	8,202	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	44,2929	0,000	0,0000	1/1
15	☑	Peak 8,597 Ca…	8,597	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	35,8476	0,000	0,0000	1/1
16	☑	Peak 8,945 Ca…	8,945	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	41,4509	0,000	0,0000	1/1
19	☑	Peak 10,383 C…	10,383	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	28,0263	0,000	0,0000	1/1
20	☑	Peak 14,878 C…	14,878	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	108,0686	0,000	0,0000	1/1

13. Rename the automatically pre-filled names in the *Calibration Summary Table* column.
14. Enter values into *Amount* column. The first concentration level is finished now. It is possible to proceed building up to next levels of calibration.

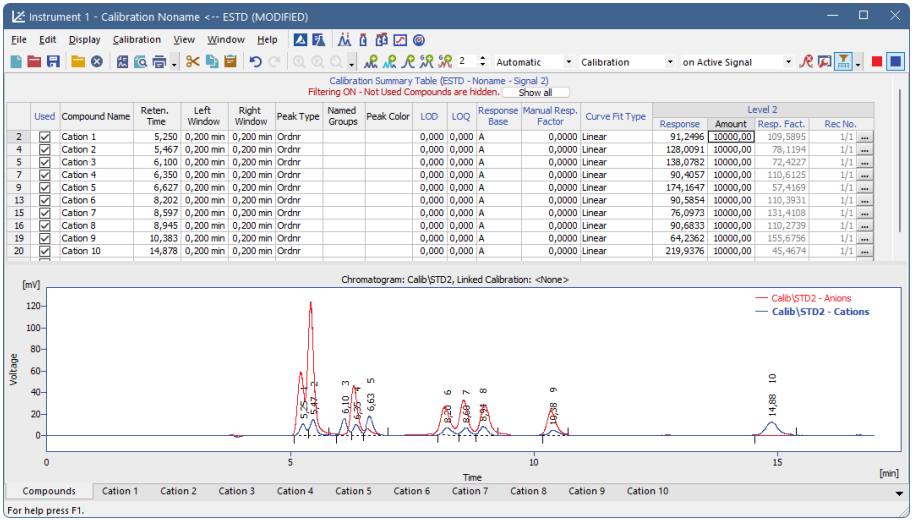
Note: All rows of *Amount* column have to be filled in.



	Used	Compound Name	Reten. Time	Left Window	Right Window	Peak Type	Named Groups	Peak Color	LOD	LOQ	Response Base	Manual Resp. Factor	Curve Fit Type	Level 1 Response	Level 1 Amount	Level 1 Resp. Fact	Level 1 Rec No.
2	☑	Cation 1	5,250	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	45,6248	5000,000	109,5895	1/1
4	☑	Cation 2	5,467	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	64,0045	5000,000	78,1194	1/1
5	☑	Cation 3	6,100	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	68,2138	5000,000	73,2990	1/1
7	☑	Cation 4	6,350	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	43,3735	5000,000	115,2779	1/1
9	☑	Cation 5	6,627	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	81,2760	5000,000	61,5188	1/1
13	☑	Cation 6	8,202	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	44,2929	5000,000	112,8849	1/1
15	☑	Cation 7	8,597	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	35,8476	5000,000	139,4794	1/1
16	☑	Cation 8	8,945	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	41,4509	5000,000	120,6247	1/1
19	☑	Cation 9	10,383	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	28,0263	5000,000	178,4037	1/1
20	☑	Cation 10	14,878	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	108,0686	5000,000	46,2669	1/1

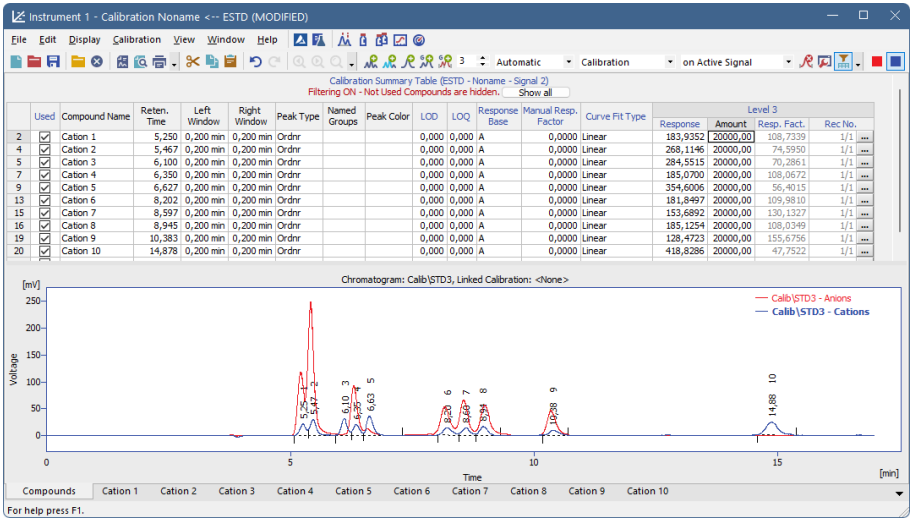
15. Open chromatogram of standard of the next (second) concentration level.
16. Fill the next level of *Calibration Summary Table* with Responses for each signal following the same steps as for Level 1 (Steps 8-16, renaming the compounds is omitted as the names carry over from previous levels).

Note: *Add Existing* can be used instead of *Add All*. This command only adds response for peaks that are preset on first level. This means that extra peaks (or peaks chosen not to be evaluated) that are present in the second (and later) standards, but not in the first one will not be added.



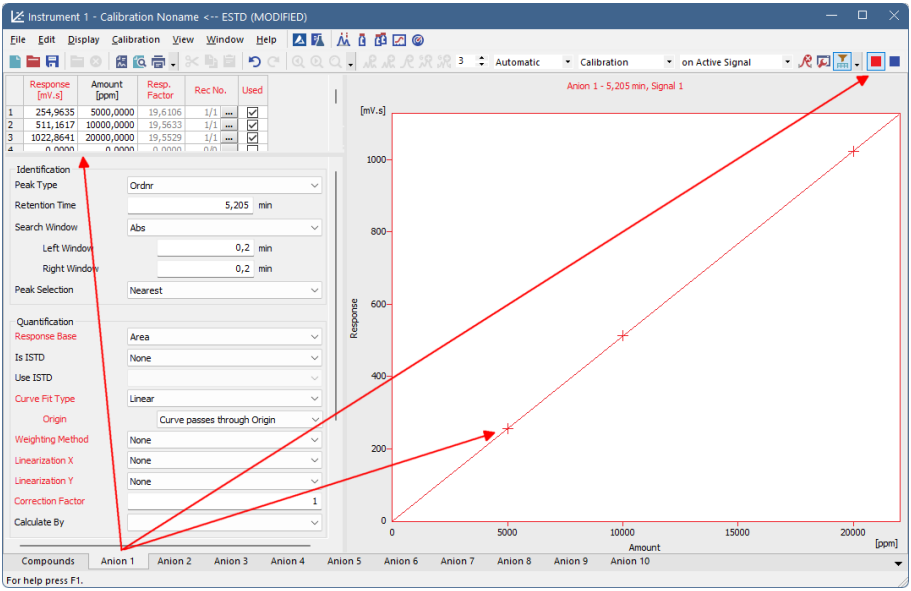
	Used	Compound Name	Reten. Time	Left Window	Right Window	Peak Type	Named Groups	Peak Color	LOD	LOQ	Response Base	Manual Resp. Factor	Curve Fit Type	Level 2 Response	Level 2 Amount	Level 2 Resp. Fact.	Level 2 Rec No.
2	☑	Cation 1	5,250	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	91,2496	10000,00	109,5895	1/1
4	☑	Cation 2	5,467	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	128,0091	10000,00	78,1194	1/1
5	☑	Cation 3	6,100	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	138,0782	10000,00	72,4227	1/1
7	☑	Cation 4	6,350	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	90,4057	10000,00	110,6125	1/1
9	☑	Cation 5	6,627	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	174,1647	10000,00	57,4169	1/1
13	☑	Cation 6	8,202	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	90,5854	10000,00	110,3931	1/1
15	☑	Cation 7	8,597	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	76,0973	10000,00	131,4108	1/1
16	☑	Cation 8	8,945	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	90,6833	10000,00	110,2739	1/1
19	☑	Cation 9	10,383	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	64,2362	10000,00	155,6756	1/1
20	☑	Cation 10	14,878	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	219,9376	10000,00	45,4674	1/1

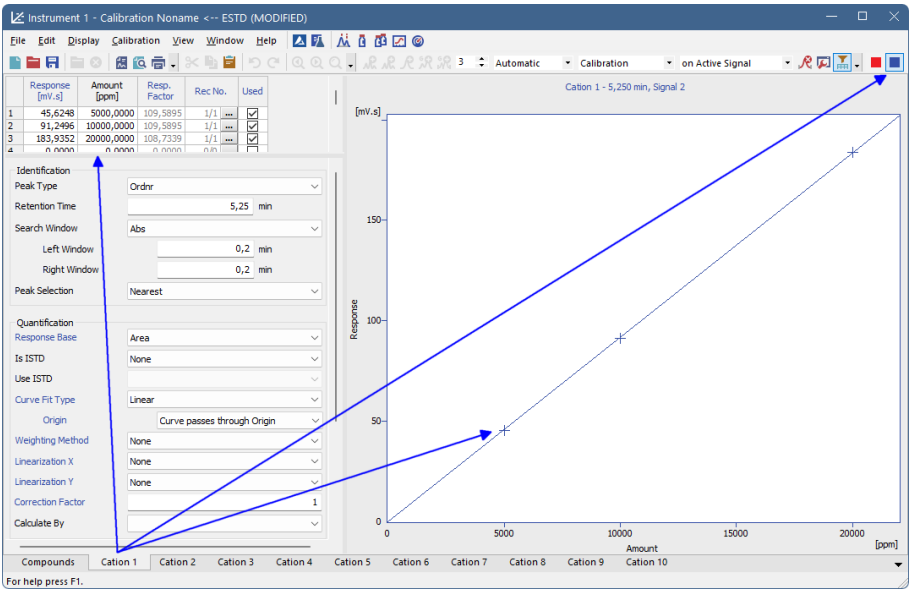
17. Open chromatogram of standard of the next (third) concentration level.
18. Fill the *Calibration Summary Table* in the same manner as for second level (step 18).



	Used	Compound Name	Reten. Time	Left Window	Right Window	Peak Type	Named Groups	Peak Color	LOD	LOQ	Response Base	Manual Resp. Factor	Curve Fit Type	Level 3 Response	Level 3 Amount	Level 3 Resp. Fact.	Level 3 Rec No.
2	☑	Cation 1	5,250	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	183,9352	20000,00	108,7339	1/1
4	☑	Cation 2	5,467	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	268,1146	20000,00	74,5950	1/1
5	☑	Cation 3	6,100	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	284,5515	20000,00	70,2861	1/1
7	☑	Cation 4	6,350	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	185,0700	20000,00	108,0672	1/1
9	☑	Cation 5	6,627	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	354,6006	20000,00	56,4015	1/1
13	☑	Cation 6	8,202	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	181,8497	20000,00	109,9810	1/1
15	☑	Cation 7	8,597	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	153,6892	20000,00	130,1327	1/1
16	☑	Cation 8	8,945	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	185,1254	20000,00	108,0349	1/1
19	☑	Cation 9	10,383	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	128,4723	20000,00	155,6756	1/1
20	☑	Cation 10	14,878	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	418,8286	20000,00	47,7522	1/1

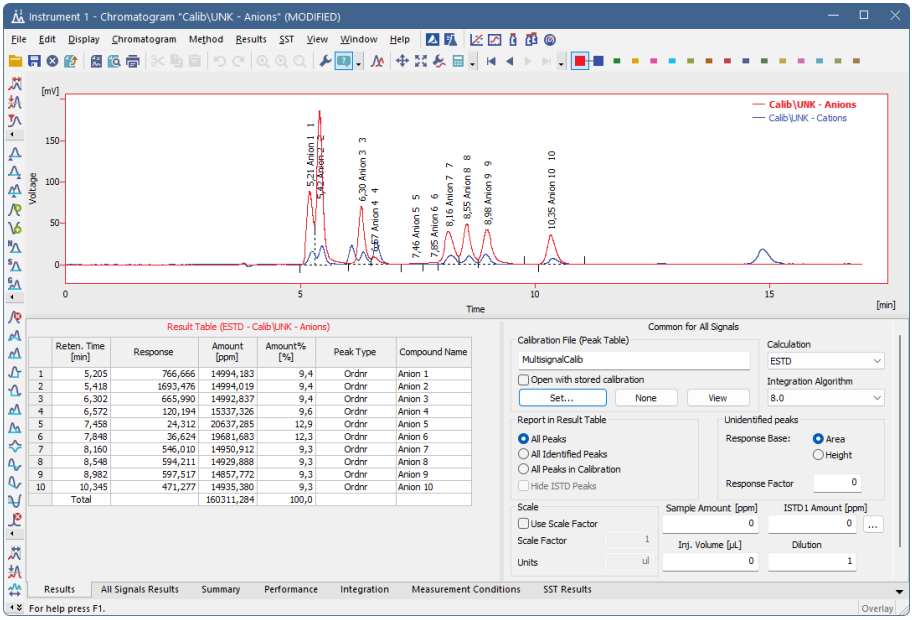
Note: It is possible to review calibration curves for each compound on the respective tabs of individual compounds. Notice that calibration curve are displayed only for valid signal (When filtering is enabled tabs of individual compounds are displayed only on signal where they are used). Signal selection is located in right upper corner of the *Calibration Window*.

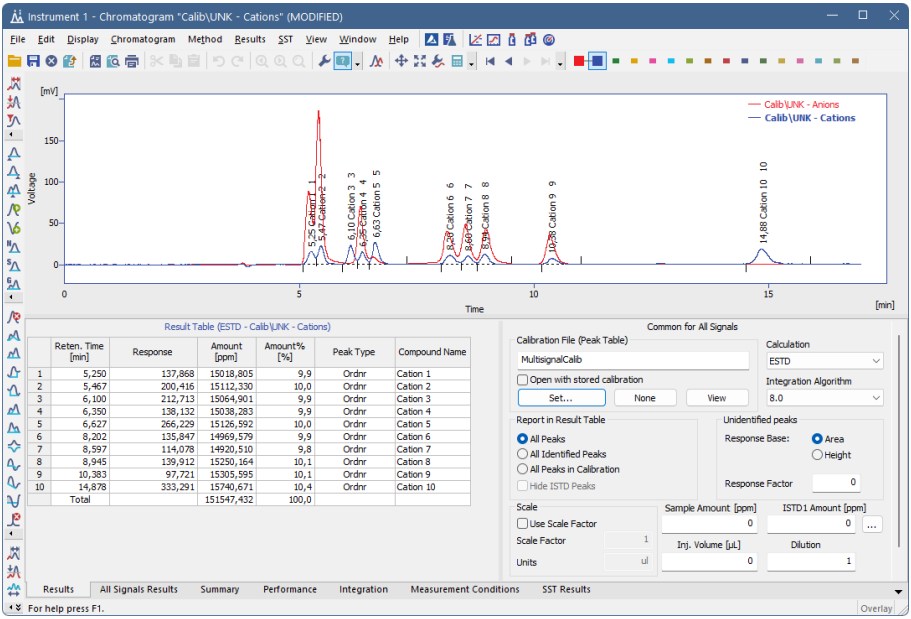


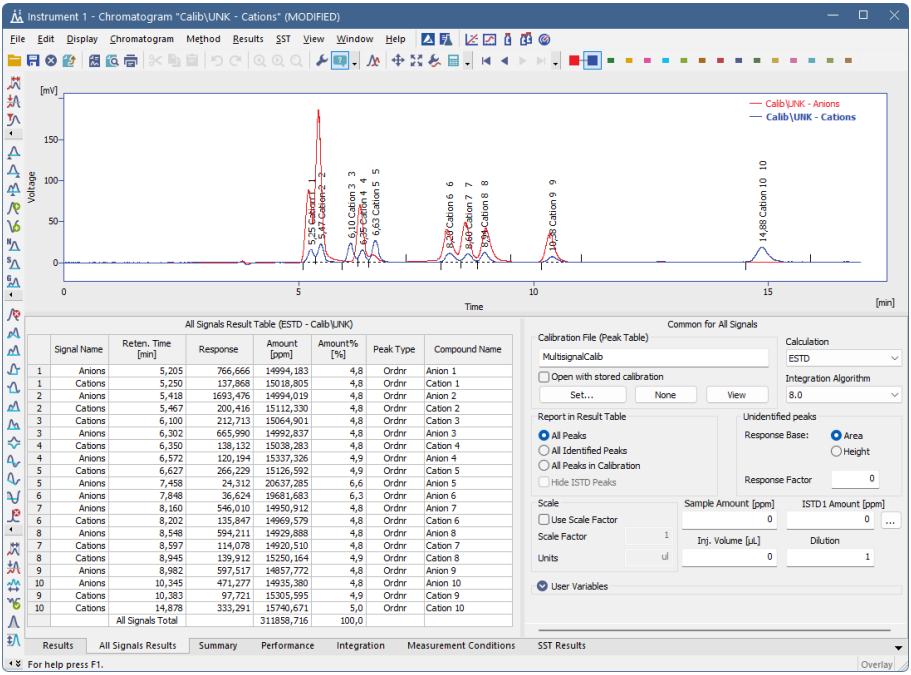


19. When calibration is finished do not forget to save it using select *File - Save* or click on .

20. For calculating result in sample open the **Chromatogram window** select *Window - Chromatogram* on the *Instrument* window or click on and open chromatogram of sample and link the calibration to chromatogram.
21. Review results on *Results Table* of each individual signal or review results for all signals on *All Signals Results* Table.




Instrument 1 - Chromatogram "Calib\UNK - Cations" (MODIFIED)
File Edit Display Chromatogram Method Results SST View Window Help
[mV]
Voltage
Time
[min]
Calib\UNK - Anions
Calib\UNK - Cations
5,25 Cation 1
5,47 Cation 2
6,10 Cation 3
6,35 Cation 4
6,63 Cation 5
8,20 Cation 6
8,49 Cation 7
8,94 Cation 8
10,38 Cation 9
14,88 Cation 10
Result Table (ESTD - Calib\UNK - Cations)
Reten. Time [min] | Response | Amount [ppm] | Amount% [%] | Peak Type | Compound Name
1 5,250 137,868 15018,805 9,9 Ordnr Cation 1
2 5,467 200,416 15112,330 10,0 Ordnr Cation 2
3 6,100 212,713 15064,901 9,9 Ordnr Cation 3
4 6,350 138,132 15038,283 9,9 Ordnr Cation 4
5 6,627 266,229 15126,592 10,0 Ordnr Cation 5
6 8,202 135,847 14969,579 9,9 Ordnr Cation 6
7 8,597 114,078 14920,510 9,8 Ordnr Cation 7
8 8,945 139,912 15250,164 10,1 Ordnr Cation 8
9 10,383 97,721 15305,595 10,1 Ordnr Cation 9
10 14,878 333,291 15740,671 10,4 Ordnr Cation 10
Total 151547,432 100,0
Common for All Signals
Calibration File (Peak Table)
MultisignalCalib
Open with stored calibration
Set... None View
Calculation
ESTD
Integration Algorithm
8.0
Report in Result Table
All Peaks
All Identified Peaks
All Peaks in Calibration
Hide ISTD Peaks
Unidentified peaks
Response Base: Area Height
Response Factor 0
Scale
Use Scale Factor
Scale Factor 1
Units ul
Sample Amount [ppm] 0
ISTD1 Amount [ppm] 0
Inj. Volume [µL] 0
Dilution 1
Results All Signals Results Summary Performance Integration Measurement Conditions SST Results
For help press F1.
Overlay



10.10.2 Using Internal Standard (ISTD) in calibration

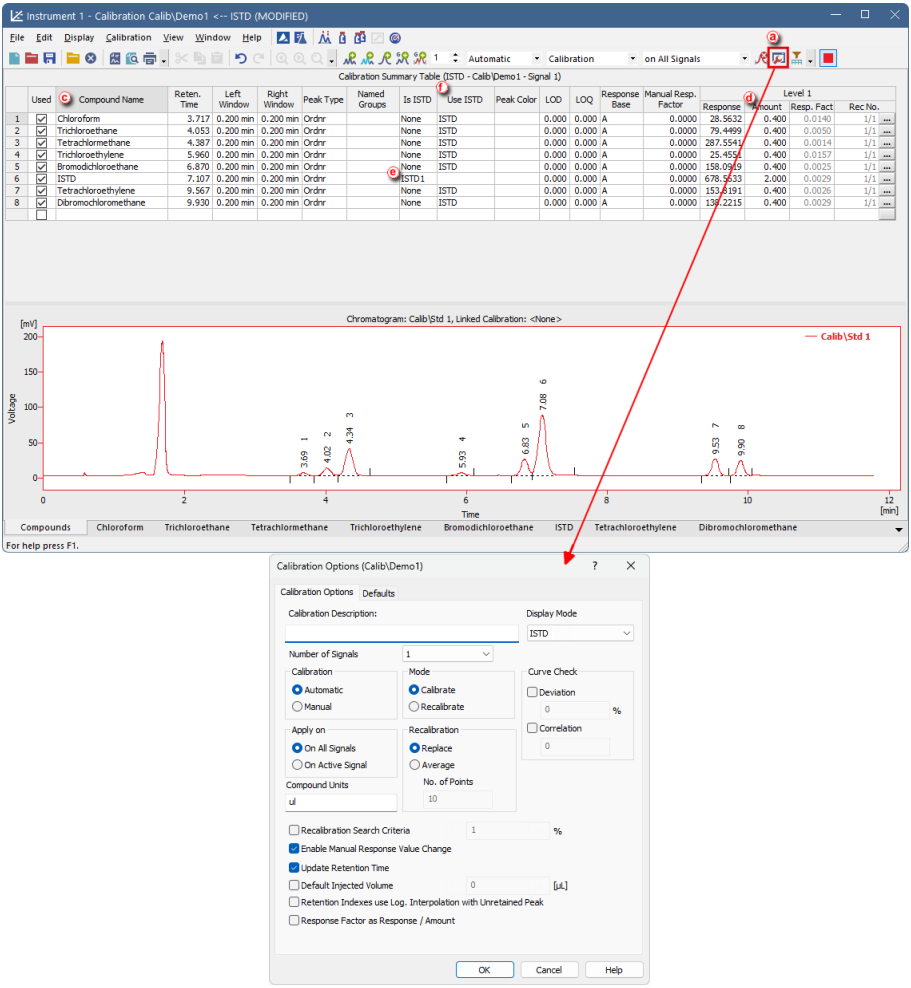
The use of internal standard (ISTD) helps to compensate for non-reproducible injected volume or for analyte losses during sample preparation. A known amount of internal standard compound (which should have similar properties as the analyte, but should not be present in the samples) is added to the standards and samples. The determined analyte amounts are then corrected based on the ratio of the added and detected amounts of the ISTD compound(s).

This chapter provides detailed insights into the differences when creating a calibration with ISTD compared to a standard calibration, as described in Creating a new calibration.

1. In the *Calibration Options* window (accessible via the icon ⓐ in the *Calibration* window), change the *Display Mode* to *ISTD* ⓑ .
2. Open your first calibration standard and add peaks to the Calibration Summary Table as usual.
3. Label the peaks by the compound names in the corresponding column ⓒ and fill in the *Amount* column ⓓ with the amounts of the present compounds including ISTD.
4. In the row corresponding to ISTD, change the type of the cell in the *Is ISTD* column to *ISTD1* ⓔ . The *Use ISTD* column ⓕ now contains the name of the

selected ISTD compound in all the other rows. In compounds tabs, the axes are labeled according to the selected ISTD.

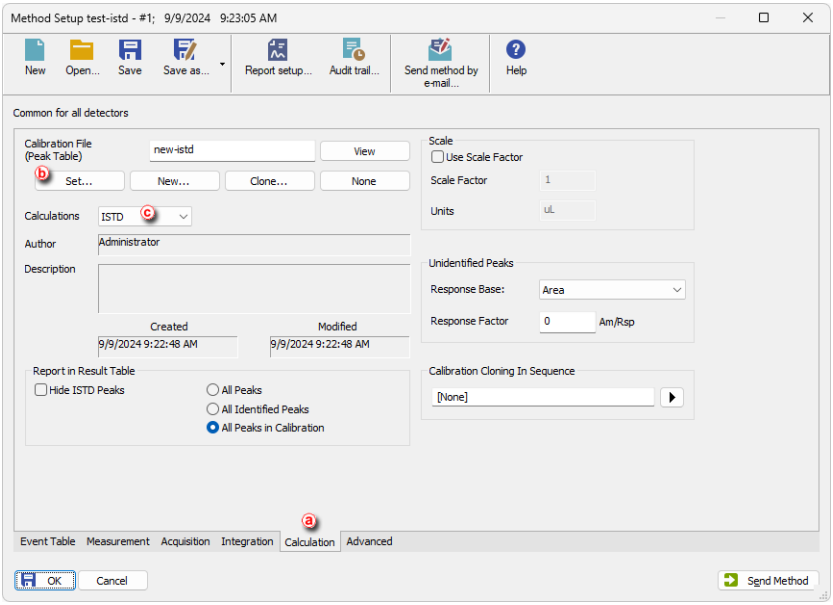
Note: You can set up to 10 compounds as ISTDs in the *Is ISTD* column. When more ISTDs are present, you can specify which one to use for quantification of which compound in the *Use ISTD* column.



5. Now, the first calibration level is set. Continue as usual to set the remaining calibration levels using the measured calibration standards (as shown in Adding a new calibration level). Enter the ISTD amounts according to the mode you plan to work in.

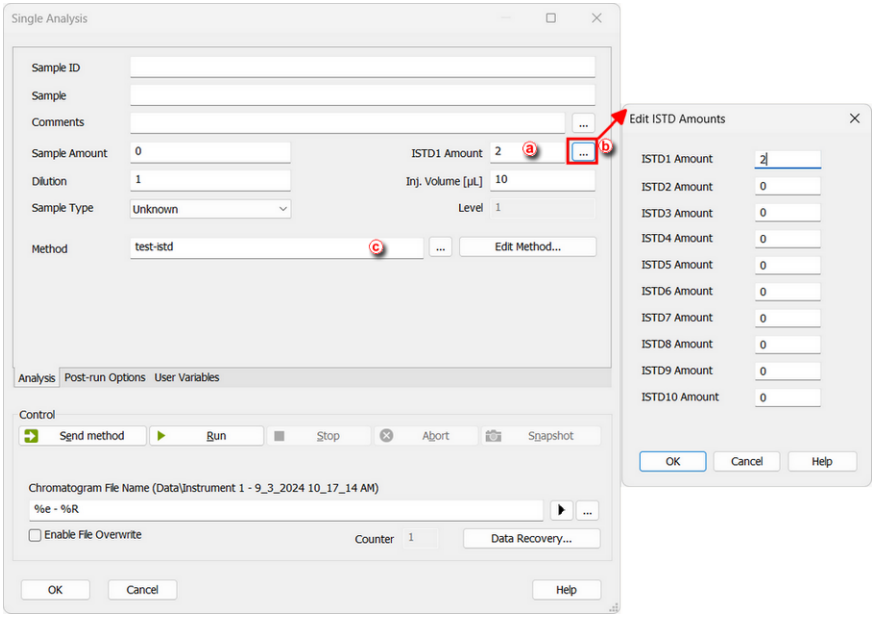
The created ISTD calibration may now be linked to an already measured chromatogram for direct results assessment (see Applying calibration to a chromatogram), and it may be also linked to a method. This causes that the chromatograms measured using this method will be automatically evaluated using the pre-selected ISTD calibration.

6. To link the ISTD calibration to a method, in *Method Setup*, open the *Calculation* tab ⓐ and set the created ISTD calibration file ⓑ. The *ISTD* parameter ⓒ should be selected in the *Calculations* option. Press the *OK* button to save the Method and close the dialog.



7. To use the ISTD method in single analysis, set the *ISTD1 Amount* ⓐ in the *Single Analysis* window to the desired value. In the case of more than one ISTD compound present, set the amounts in the dialog which opens by clicking the triple dot ... menu ⓑ.

8. Select the previously created method ⓒ. You can *Run Acquisition* directly from the *Single Analysis* window.



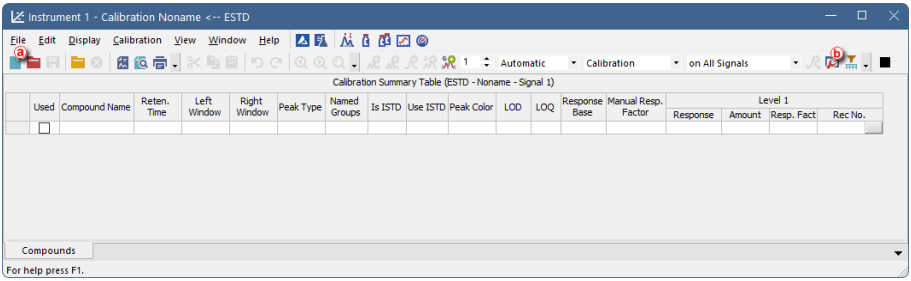
The sequence analysis setup is analogous to the single analysis. The ISTD2–ISTD10 amount columns are not shown by default and can be added via the *Edit - Setup columns...* dialog.

Note: In the case the amount of internal standard is the same for all standards and samples, it is possible to enter zero instead of the amount (which may not be known). In such case, the correction will be based on the ratio of the ISTD peak response in the standards and unknowns. Note that the ISTD amounts must be entered or set to zero both in Calibration and in the Sample Header. A mismatch will be detected and reported as error.

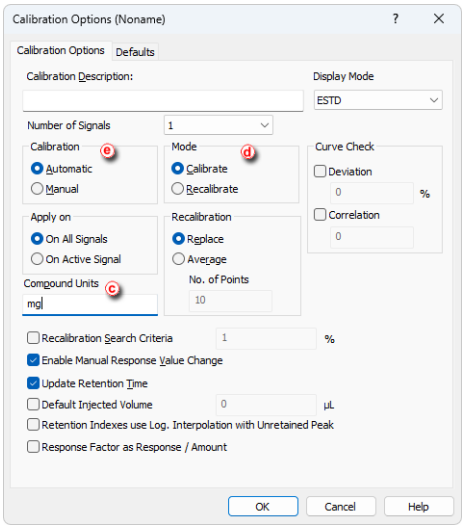
10.10.3 Calibrating with manually entered Response Factors

When using a free calibration, the amounts for each component are calculated using the *Response Factor* instead of a calibration curve.

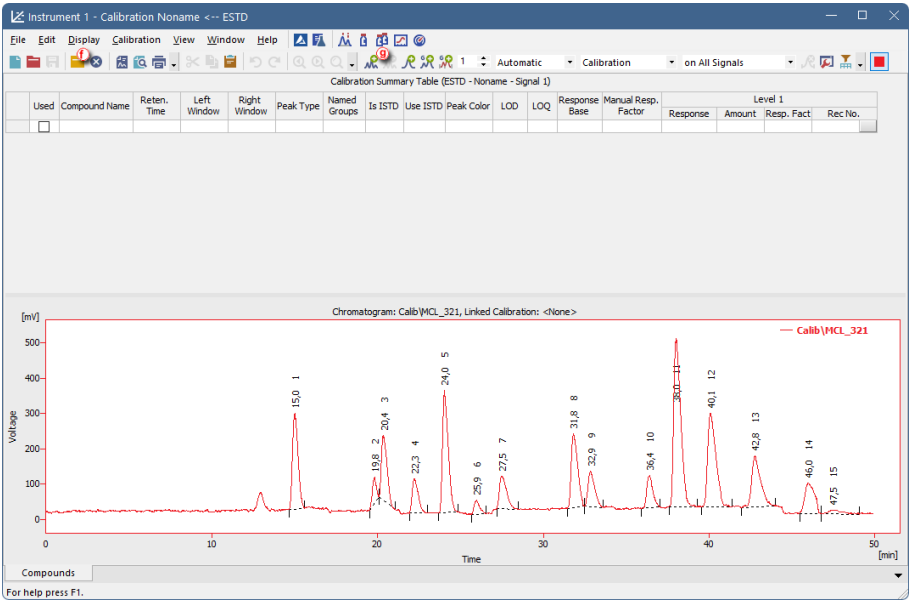
1. Create a new calibration file: select *File - New* or click ⓐ .



2. Open the Calibration Options dialog: choose *Calibration - Options…* or click . ⓑ



3. Check that the *Compound Units* ⓒ are set correctly, *Mode* to *Calibrate* ⓓ and *Calibration* option is set to *Automatic* ⓔ .
4. Open an integrated chromatogram of a standard (containing peaks of compounds of interest with a known concentration): select *File - Open Standard…* or click ⓕ on the *Calibration* window.
5. Add all peaks in the chromatogram of the calibration standard to the calibration file. Choose *Calibration - Add All* or click on ⓖ .

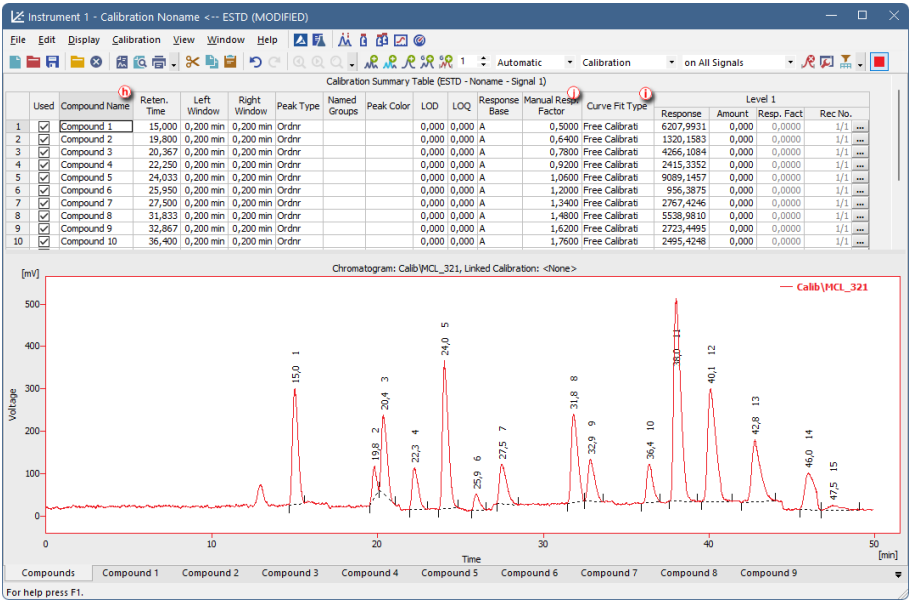


6. Name the peaks identified in the *Calibration Summary Table* ⓗ by their retention times by typing the *Compound Name* for each peak. No peak name may be used more than once.
7. Set the *Calibration Fit Type* to *Free Calibration* ⓘ for each one of the compounds in the *Calibration Summary Table*.

   More Info:

   Right click on the table and select the option *Set Columns...* to add the *Calibration Fit Type* column to the table. Alternatively, you can click on each compound tab at the bottom of the *Calibration* window and set the *Calibration Fit Type* from there.

8. Type in the *Manual Response Factor* for each one of the compounds ⓙ .



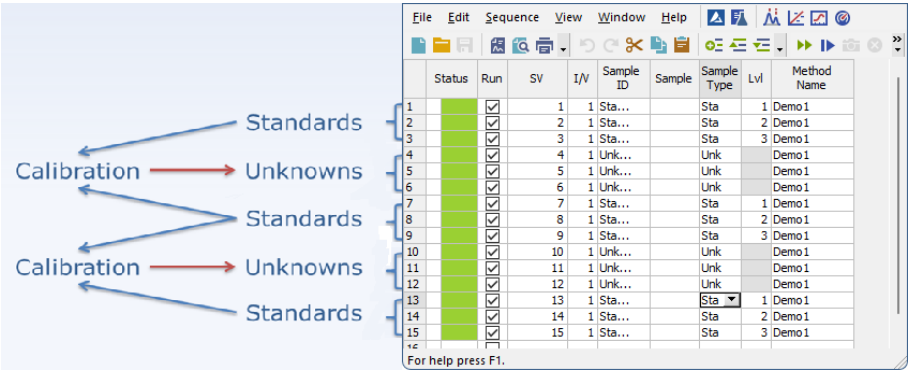
Caution: Calibration curve cannot be constructed when amount is set to zero for all levels. In case calibration curve could not be constructed for one of the compounds, no results are calculated for all of the compounds (as the total amount could be wrong). If you do not want to calculate amounts for all identified compounds, you could use free calibration with zero response factor.

10.10.4 Compensating for response drift using bracketing

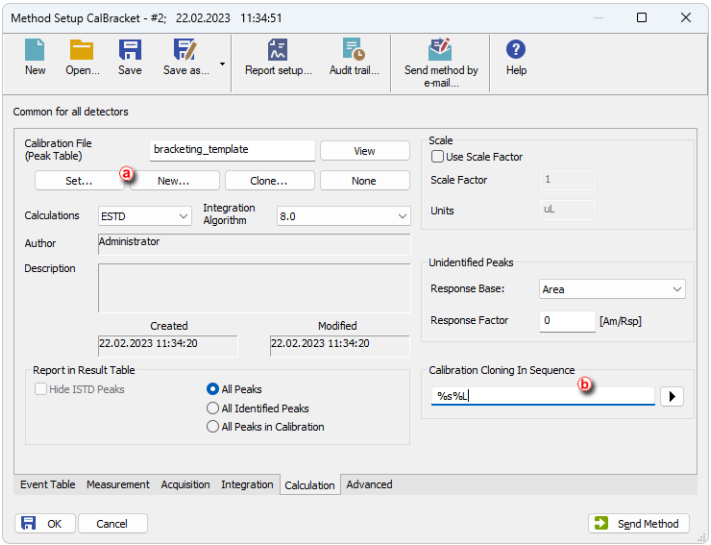
Bracketing is a direct calibration method used to compensate for the variation in instrument response with time. Typical use is for detector response deteriorating or sample containing compounds staining or interacting with the column. Bracketing is not helpful for random variations. Bracketing may be in place when 2 calibration curves measured on the same series of standards have a stable trend and good correlation, but they are not the same.

To use bracketing in sequence, the order of the rows must be standards, then unknowns, then standards again. Usually, two standards are used; more standards could be used if the measuring instrument has a non-linear response. Samples are evaluated by a calibration which is created by averaging the standards before and after the unknown. As every unknown sample series is demarcated by calibration standards it uses a single calibration. Calibration will be cloned from the previous calibration clone whenever an unknown sample or blank follows the calibration standard. The newly cloned calibration file has all responses cleared - apart from the responses from the last series of calibration standards (immediately preceding the current unknown samples).

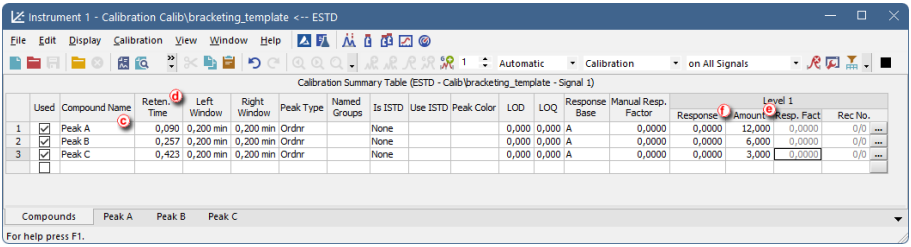
Bracketing in Clarity

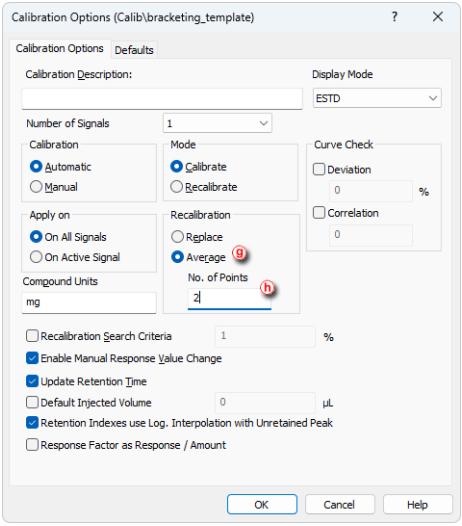


1. Open the method that will be used in the sequence: click *File - Open Method…* from the *Instrument* window.
2. Navigate to *Calculation* tab.
3. Set the template calibration as Calibration File: click *Set...* ⓐ and select the calibration. Note that this calibration will remain unchanged, newly created clone of the calibration will be used with new responses.
4. Set the name of the cloned calibration: set the name in *Calibration Cloning In Sequence* ⓑ. You can use predefined parameters (refer to ***Creating customized file names automatically***).



5. Click *OK* and save the modified method.
6. Open Calibration window and the template calibration: click *Window - Calibration* from the *Instrument* window and *File - Open...* in the *Calibration* window, select the template calibration (in this case bracketing_ template.cal).
7. Set *Compound Names* ⓒ , *Retention Time* ⓓ , *Amounts* ⓔ , etc., but no *Responses* ⓕ (you can use previously measured standard to get the Retention Times).
8. Update *Calibration Options*: Set *Recalibration* to *Average*ⓖ and *No. of Points* to 2ⓗ (no more points needed as they would not be applied anyway).
9. Save changes and close the calibration.

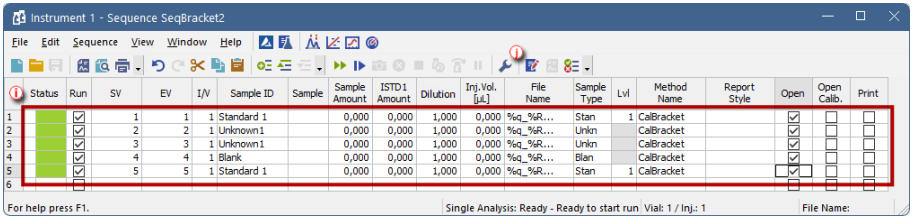




10. Open *Sequence* window and create a new sequence: click *Analysis - Sequence* and then icon.
11. Set the sequence according to the following steps: (for more details about creating the sequence refer to ***Creating and running a sequence***)
    - Set the row/s for the standard/s. ⓘ
    - Add a row for a blank, if you wish to.
    - Set the row/s for the unknown samples.
    - Repeat the row/s for the standard/s.

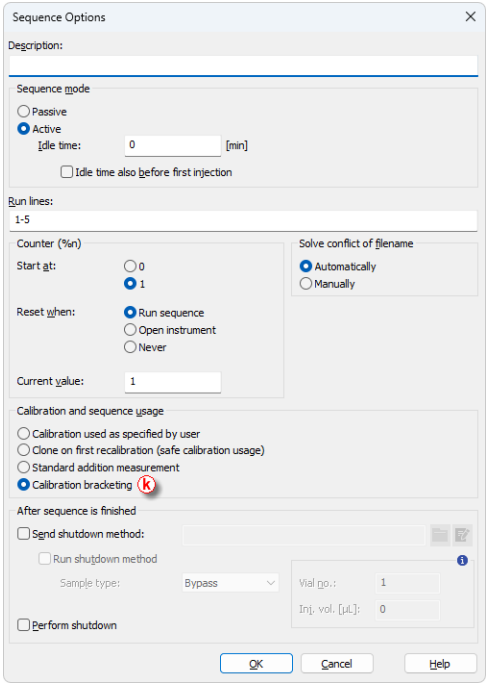
Note: The sequence must start and end with a row with *Standard Sample Type*.

- Repeat the previous four steps for every "bracket" of unknown samples you wish to add.



12. Set the sequence to operate in the calibration bracketing mode:
    - Click icon to open the *Sequence Options* dialog. ⓙ
    - Check *Calibration Bracketing*. ⓚ
    - Click *OK*.

Note: If your sequence is using multiple methods, calibration using bracketing is still possible to use but make sure that the Calculation tab is exactly the same for all the methods used in the sequence.



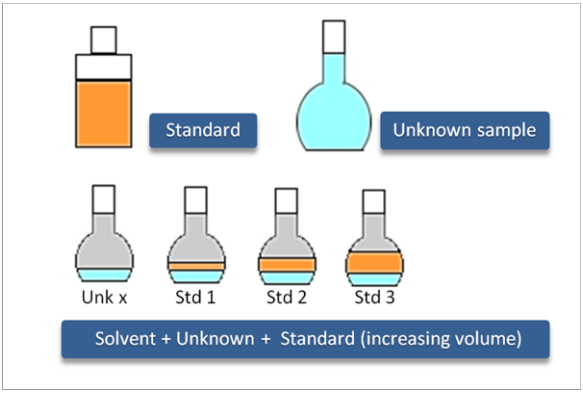
13. Run the sequence (for more details about running the sequence refer to *Creating and running a sequence)* .
14. The results shown while the sequence is running are recalculated at the end of each bracket, when the standard after the unknown sample is acquired.

The calibration used is an average of the two calibrations, before and after the unknown.

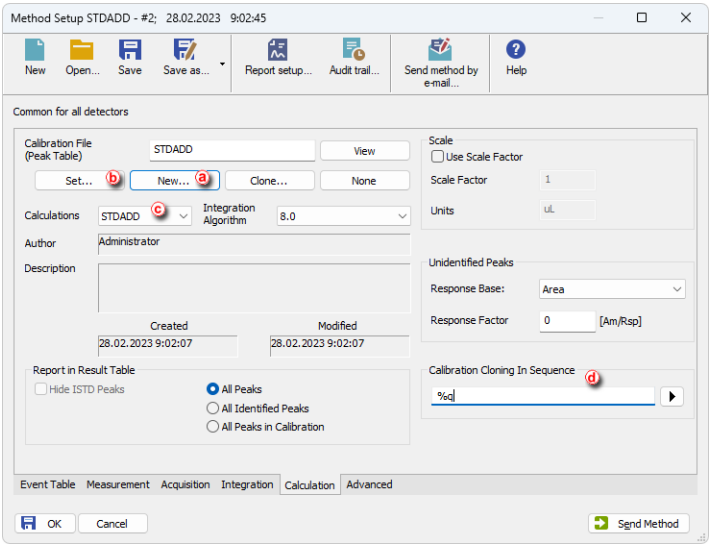
Note: The measured sequence can be reprocessed using Batch. For more info see the topic Reprocessing whole sequence while using calibration cloning.

10.10.5 Improving quantification with the standard addition method

Standard addition is a quantification approach (similar to ESTD or ISTD) useful in case the sample matrix is complex and when it influences responses of analytes. By spiking samples with a series of increasing amounts of the analytes, standard addition calibration curves for each sample are obtained from which the concentrations of unknown samples can be calculated.



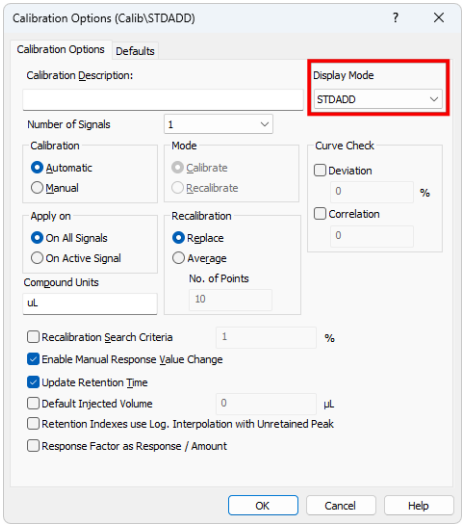
1. Create a new method or open your already prepared method. Go to *Method Setup - Calculation* tab.
2. Create *New* calibration file ⓐ or *Set* your already created Calibration file ⓑ .



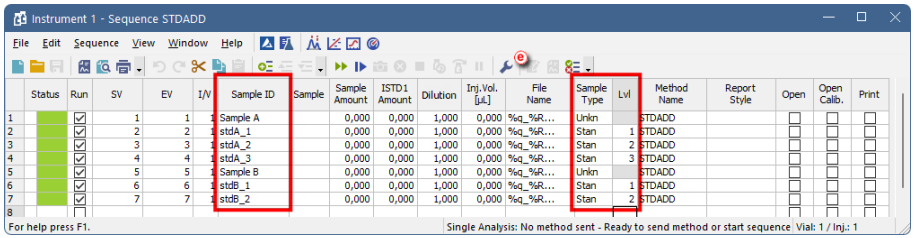
3. Select *STDADD* in the *Calculations* drop-down list ⓒ .
4. Create a custom name for the cloned calibration files in *Calibration Cloning in Sequence* ⓓ and click *OK*.

> *Note:* Make sure that each of the measured samples will have a unique calibration name; use predefined parameters to achieve that.

5. Open the *Calibration* window by selecting *Window - Calibration* in the *Instrument* window.
6. Open the *Calibration Options* dialog. Choose *Calibration - Options…* or click on . Select the *STDADD* in the *Display Mode* drop-down list and click ***OK***.

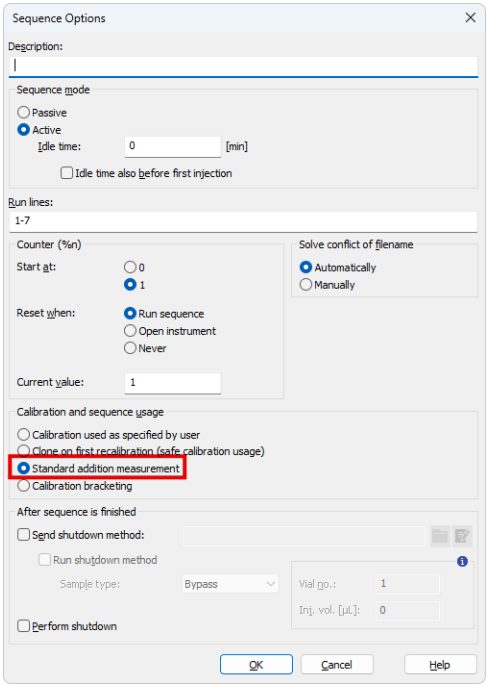


7. Create a new sequence with the given order of the lines:
   - Sample A
   - Sample A with Standard level 1
   - Sample A with Standard level 2
   - Sample A with Standard level X
   - Sample B
   - Sample B with Standard level 1
   - Sample B with Standard level X
   - *continue with the given pattern until desired state*
8. Set the columns as follows: for Unknown samples set *Sample Type* column to *Unknown* and for Standard Addition samples, set *Sample Type* column to *Standard* and *Lvl* column to level corresponding to the added amount in given sample.

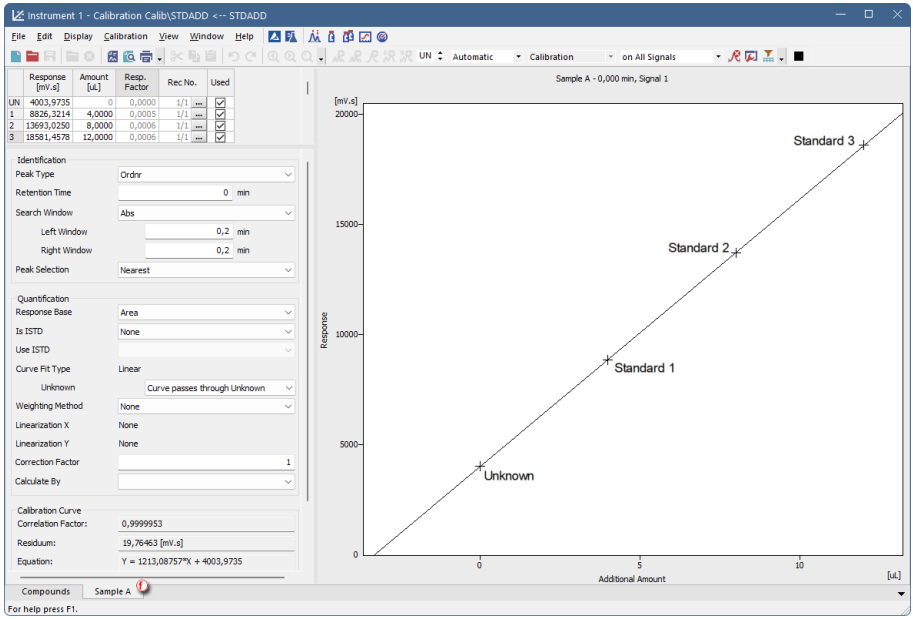


Note: In case you want to use a blank sample too, such sample shall be always put in the sequence before the unknown sample.

9. Click to open the *Sequence Options* dialog ⓔ and select *Standard Addition Measurement* and click *OK*.



10. Run the sequence and wait until the sequence is finished.
11. Open the *Calibration* window: choose *Window* - *Calibration* in the *Instrument* window or click on .
12. Go to *File* - *Open* and open the cloned calibration file for the desired sample.
13. Click on the *Compound* tab ⓕ to see the calibration curve. Fill in the amounts of the standard samples.



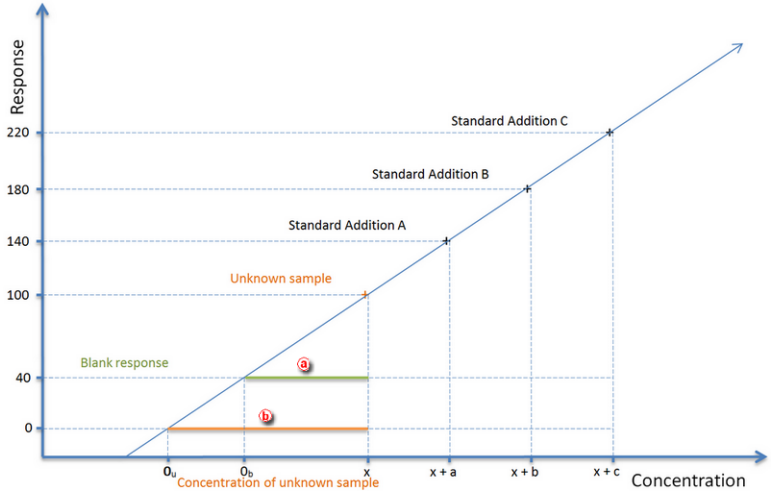
14. Open chromatogram of the desired unknown sample. The Result Table now contains amount of the unknown sample, calculated using Standard Addition.

Note: The measured sequence can be reprocessed using Batch. For more info see the topic Reprocessing whole sequence while using calibration cloning.

10.10.5.1 How the concentration is calculated

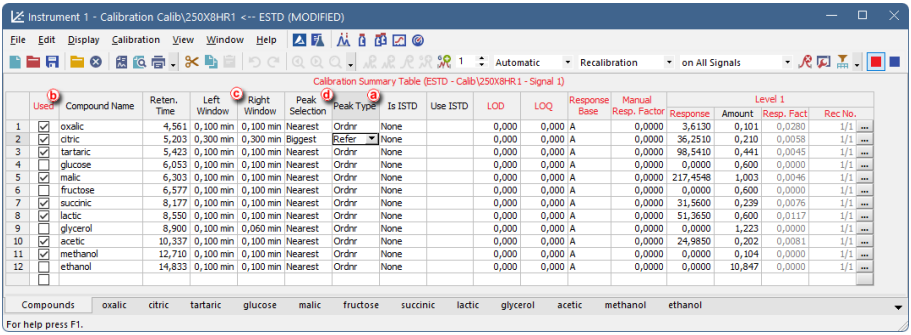
The concentration of an unknown sample is calculated using a calibration curve, which intersects in the point [0,0].

As shown in the picture below, when not using Blank samples the the concentration of an unknown sample equals the orange line (0 response corresponds to 0 unknown sample concentration - 0u), whereas the concentration of the UNKNOWN SAMPLE when using Blank equals the green line (Blank response corresponds to 0 unknown sample concentration - 0b).



10.10.6 Using a reference peak to improve compound identification

A reference peak is a peak used as a reference for recalculating the retention times for the rest of the peaks in a chromatogram. This method allows a better compound identification in those cases where there might be a drift in the retention times in repeated analyses. It is possible to set multiple reference peaks. For ordinary peaks, the expected retention times will be adjusted by linear interpolation between the nearest reference peaks.



1. Open the calibration file: choose *File - Open…* or click on .
2. Select *Refer* on the *Peak Type* column for an easily identifiable compound (i.e. main compound, ISTD standard, any well resolved peak of the matrix) that you will use as a reference ⓐ . To apply the reference peak, *Used* check-box must be checked ⓑ .

3. Edit the Left and Right window values to define the range within which the peak should appear ⓒ. This window may include other peaks if the selected reference peak meets the *Peak Selection* criteria.
4. Select the Peak Selection criteria: biggest, nearest, first or last peak ⓓ.

More Info:

Ordinary peaks are identified by the nearest option by default. For reference peaks the biggest will be set as default. Note that the biggest refers to the selected Response Base, i.e. if the Area is the Response Base, the detected peak may not be the highest one. In specific cases selecting First or Last may be advantageous.

To add the *Peak Selection* column:

- Right click anywhere on the table
- Select *Set Up Columns* to open the relevant window.
- Select *Peak Type* on the right and click on *Show* and then *Ok*.

5. Repeat steps 3 to 5 to add more reference peaks.

Note: In case of multisignal calibration, where compound used as reference does not match the selection criteria on some signal(s), create a variant of the compound only for that signal(s). The name must be different - e.g. Oxalic - UV, Oxalic - RI), copy the rest of the original row, check the used checkbox only for one variant on each signal. Now change the Peak Selection criteria value, or if suitable, change the Peak type to Ordinary, and select other Reference peak on that signal.

6. Save the calibration file: choose *File - Save* or click .
7. Link the calibration to your chromatogram as explained in *Applying a calibration to a chromatogram*.

10.10.7 Using Calculate By to determine the amount of a compound with no standard available

When no standard of a compound is available and a compound with known response ratio to the unavailable one is present within the sample (this information can be found in respective norm etc.) the *Calculate By* and *Correction factor* can be used to determine its amount in the sample.

1. Open the calibration file.
2. The *Calculate By* and *Correction Factor* are hidden by default. To display them right-click the table, select *Setup Columns...*and in the following dialog move the respective items from *Hide Columns* list to *Show Columns* list.
3. For compound (Chloroform in the example) ⓐ that should be evaulated by another one, select its *Calculate By* field ⓑ and pick which compound to use for the calculation (Trichloroethane in the emxaple).

Note: Only compounds (peaks) already added to the calibration can be selected.

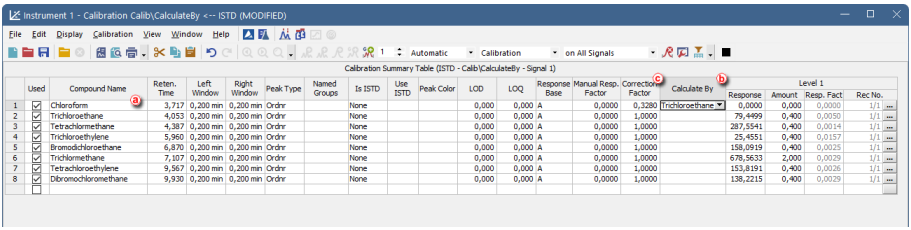
4. Fill the known response ratio to the *Correction Factor* column ⓒ.

Note: The *Amount* filled in the row that will be calculated using calibration curve of another compound will be ignored.

5. The resulting amount in *Chromatogram Results Table* will be calculated according to the calibration curve of compound selected to *Calculate By*, and multiplied by the *Correction Factor*.

Note: A compound marked as *ISTD* should neither be used as a compound that is used to calculate another compound nor as a compound that is calculated using another compound.

In the example Chloroform is calculated based on the calibration curve of Trichlorethane, their response ratio is 0.328.



10.10.8 Normalized Area % Calculation

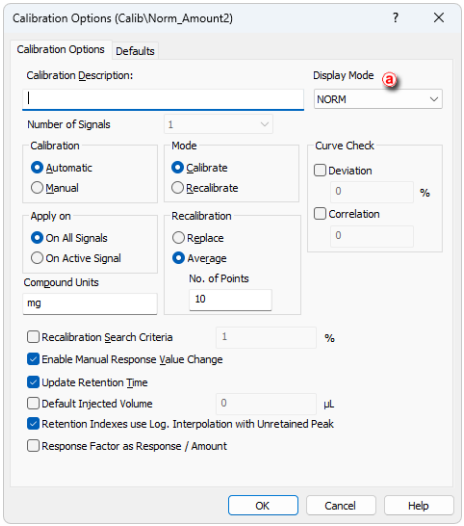
For Normalized Area % calculation no specific settings are necessary, the calculation results are always present in the *Area%* column in the Result table.

10.10.9 Normalized Amount % Calculation

This topic describes how to use Clarity, in order to obtain correct results calculated according to normalization calibration method. The normalization can be achieved by two means. First option is applicable to known response factors specific for each analyte. Second option is to use calibration based on standard sample with known fraction composition. In the latter case, Clarity automatically calculates response factors for all analytes that are subsequently applied in evaluation of the unknown sample. The results are displayed in *Amount%* column in the *Summary Table* and represent percent fraction of each analyte present in the unknown sample.

For both options set the calibration to the NORM Display mode, this ensures that Clarity checks that all the peaks are used for calculations and 100% Amount really corresponds to the whole sample.

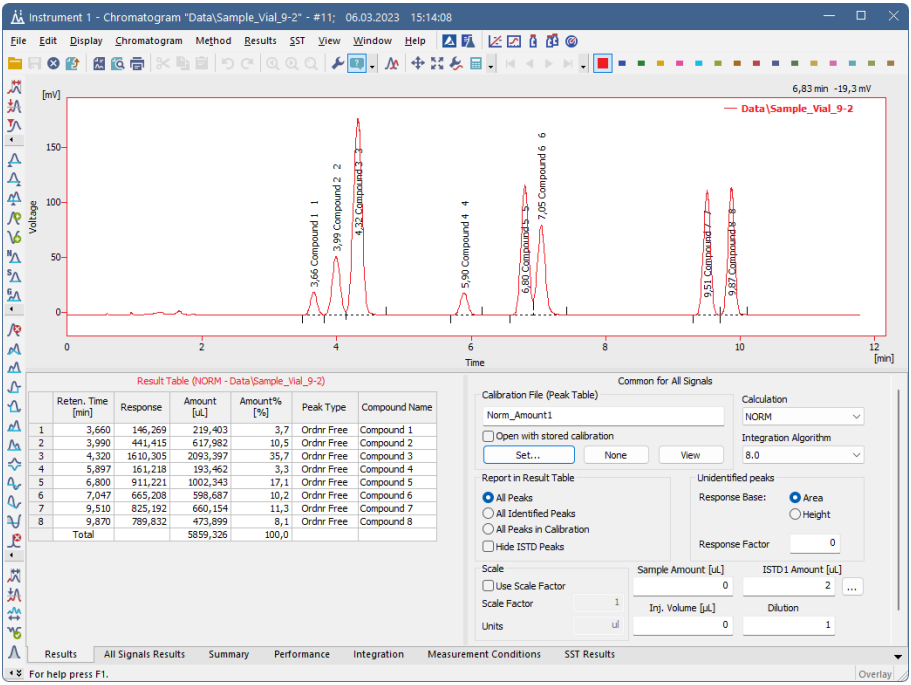
- Set *Display Mode* to *NORM* ⓐ in *Calibration Options* dialog.



A) Application of specific Response Factors

- Use procedure explained in the chapter Calibrating with manually entered Response Factors.

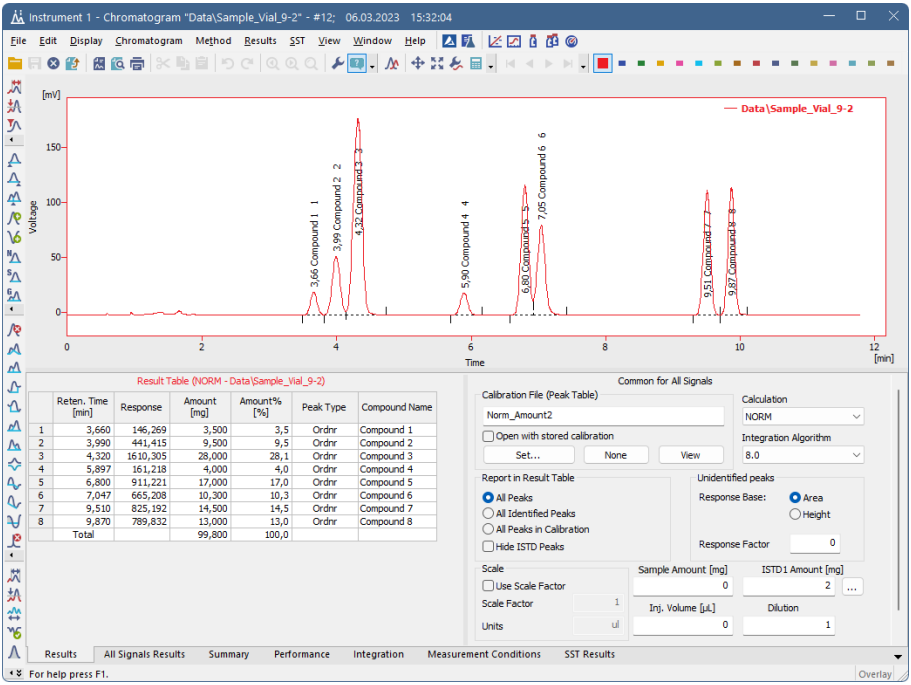
Figure below displays *Result Table* of a chromatogram with linked calibration that was created using the above mentioned method. Note different values in columns *Area [%]* and *Amount%* are caused by various values in *Manual Response Factor* column.



B) Application of automatically calculated Response Factors based on calibration with standard sample with known composition

- Use procedure explained in the chapter Creating a new calibration.

Figure below displays *Result Table* of a chromatogram with linked calibration that was created using the above mentioned method. Note different values in columns *Area [%]* and *Amount%* are caused by calculated values in *Response Factor* column.

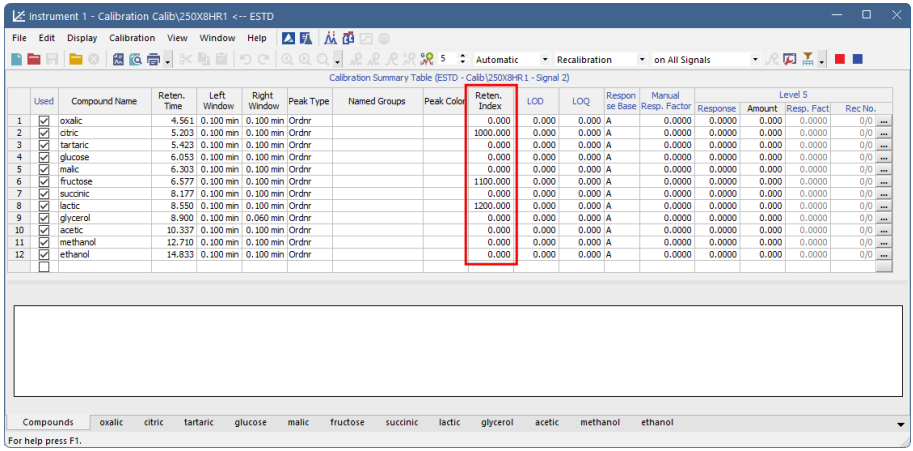


10.10.10 How to use Kováts Retention Indexes

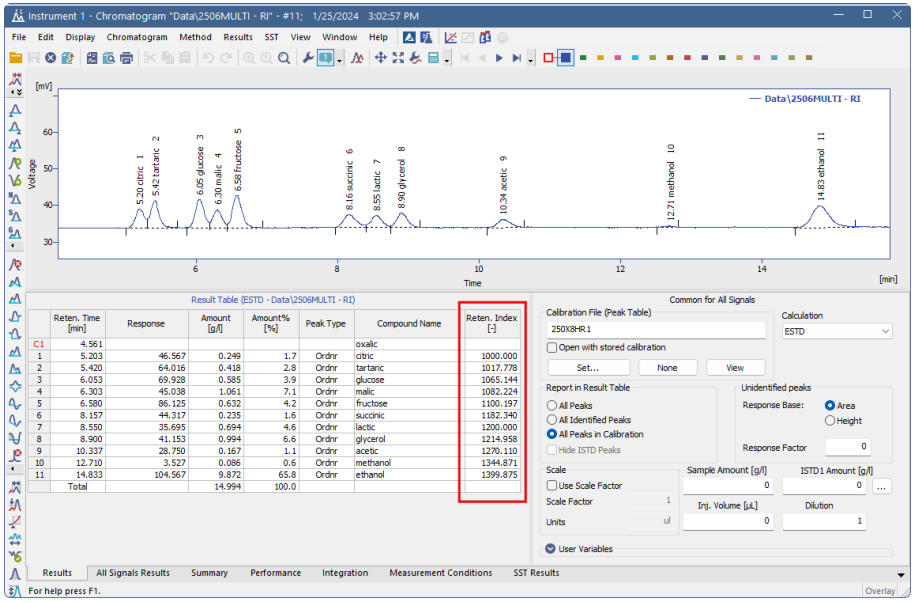
The Kováts Retention Index (*Retention Index* in **Clarity**) is used to convert the retention times of organic compounds into system-independent constants. This allows for the comparison of values measured under different conditions, such as varying column lengths, diameters, and pressures. Consequently, compound identification becomes more feasible. Kováts retention indexes are obtained by logarithmic interpolation of adjusted retention times (or volumes) using *n*-alkene standards.

To set the indexes in calibrations, follow these steps:

1. Prepare your calibration as usual.
2. The *Reten. Index* columns are hidden in the default table layout. To display them, right-click the *Calibration Summary Table* and select the *Setup Columns...* option. In the *Setup Columns* dialog, move the *Reten. Index* item to the *Show Column* list and click OK.
3. Fill in the *Retention Indexes* of the corresponding compounds. The values for the rest of the compounds may remain zero.
4. Save the calibration.

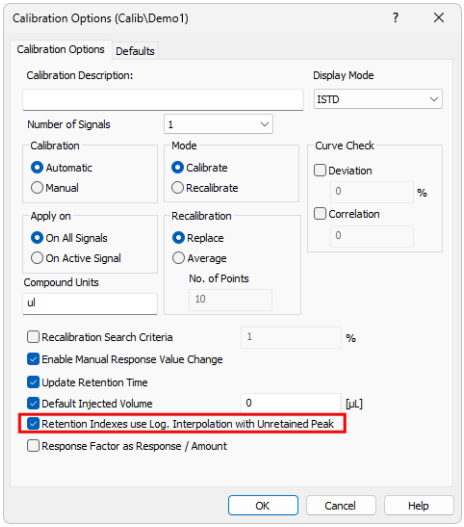


5. Open the desired chromatogram and link the created calibration. Display the *Reten. Index* columns by right-clicking in the *Result Table*, selecting *Setup Columns...*, and moving the *Reten. Index* item to the *Show Column* list in the *Setup Columns* dialog.
6. The *Result Table* will contain the retention indexes calculated according to the calibration.

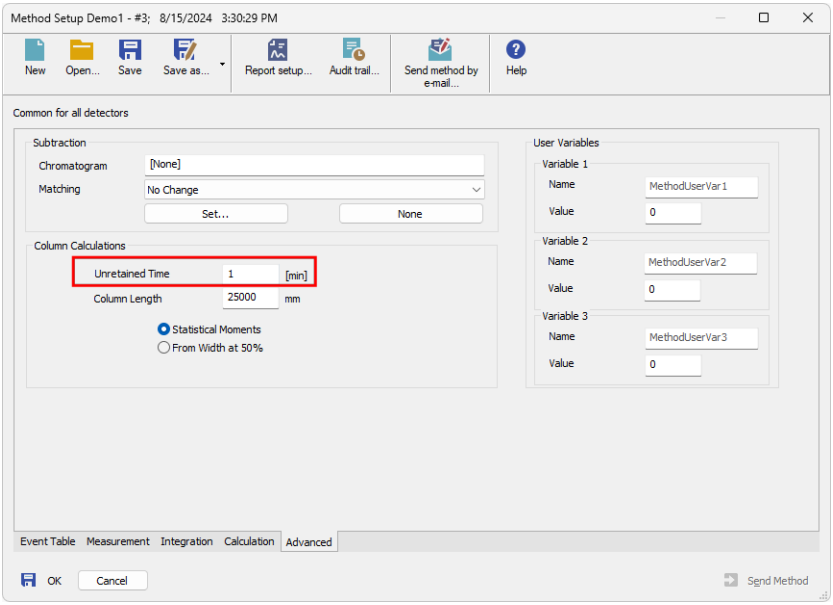


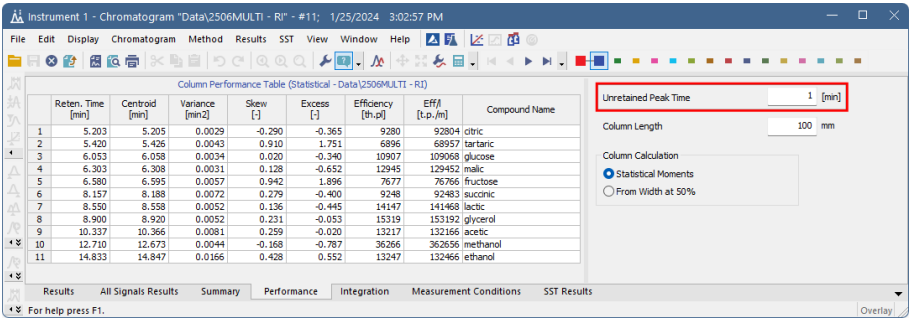
The *Unretained Peak Time* can be used for adjusting the retention times for more precise calculation of retention indexes:

1. In the *Calibration* window, open the *Calibration Options* dialog (using the *Calibration - Options...* command or the icon).
2. Retention indexes are calculated according to the selection of the *Retention Indexes use Log. Interpolation with Unretained Peak* option. If this option is **not** checked, retention indexes are calculated using linear interpolation. If it **is** checked, logarithmic interpolation with unretained peak time is used. Keep this option checked to allow for calculation using the unretained peak time.



3. The *Unretained Peak Time* may be entered in the *Method Setup - Advanced* tab, or directly in the chromatogram on the *Performance* tab.


Method Setup Demo1 - #3; 8/15/2024 3:30:29 PM
New
Open...
Save
Save as...
Report setup...
Audit trail...
Send method by e-mail...
Help
Common for all detectors
Subtraction
Chromatogram
[None]
Matching
No Change
Set...
None
Column Calculations
Unretained Time
1
[min]
Column Length
25000
mm
Statistical Moments
From Width at 50%
User Variables
Variable 1
Name
MethodUserVar1
Value
0
Variable 2
Name
MethodUserVar2
Value
0
Variable 3
Name
MethodUserVar3
Value
0
Event Table
Measurement
Integration
Calculation
Advanced
OK
Cancel
Send Method


Instrument 1 - Chromatogram "Data\2506MULTI - RI" - #11; 1/25/2024 3:02:57 PM
File
Edit
Display
Chromatogram
Method
Results
SST
View
Window
Help
Column Performance Table (Statistical - Data\2506MULTI - RI)
Reten. Time [min]
Centroid [min]
Variance [min2]
Skew [-]
Excess [-]
Efficiency [th.pl]
Eff/l [t.p./m]
Compound Name
1 5.203 5.205 0.0029 -0.290 -0.365 9280 92804 citric
2 5.420 5.426 0.0043 0.910 1.751 6896 68957 tartaric
3 6.053 6.058 0.0034 0.020 -0.340 10907 109068 glucose
4 6.303 6.308 0.0031 0.128 -0.652 12945 129452 malic
5 6.580 6.595 0.0057 0.942 1.896 7677 76766 fructose
6 8.157 8.188 0.0072 0.279 -0.400 9248 92483 succinic
7 8.550 8.558 0.0052 0.136 -0.445 14147 141468 lactic
8 8.900 8.920 0.0052 0.231 -0.053 15319 153192 glycerol
9 10.337 10.366 0.0081 0.259 -0.020 13217 132166 acetic
10 12.710 12.673 0.0044 -0.168 -0.787 36266 362656 methanol
11 14.833 14.847 0.0166 0.428 0.552 13247 132466 ethanol
Unretained Peak Time
1
[min]
Column Length
100
mm
Column Calculation
Statistical Moments
From Width at 50%
Results
All Signals Results
Summary
Performance
Integration
Measurement Conditions
SST Results
For help press F1.
Overlay

11 Batch Processing

This chapter focuses on processing more chromatograms using *Batch* dialog. There are 3 main ways of workflow Reprocessing whole sequence, Reprocessing by Method, and Post-run Options. All will be explained in more detail in this chapter.

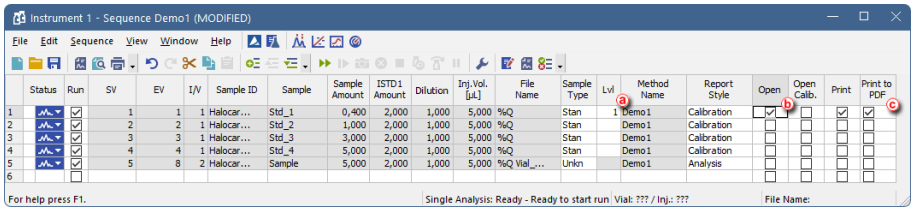
Clarity Tips&Tricks videos covering Batch topics can be found in Clarity Batch playlist.

11.1 Reprocessing whole sequence

Reprocessing whole sequence can be convenient if performing reintegration, recalibration, or changing types of samples is needed. It can also be used with calibration cloning, more in the topic Complete processing with calibration cloning. Steps below described process where sequence is already measured by template method with optimized integration parameters, for more see Save Method as a Template.

1. Measure the sequence with no post-run options set and/or no *Levels* for standards filled in (Typically, you want to perform the recalibration/export/print of the results after reviewing the chromatograms).
2. Review the chromatograms: check the integration, etc.
3. Go to the measured sequence, set *Levels* ⓐ for calibration standards and enable any post-run options you wish to perform, e.g., *Print To PDF* ⓒ . It is also possible to uncheck (check) the *Run* checkbox at rows you do not want to reprocess.

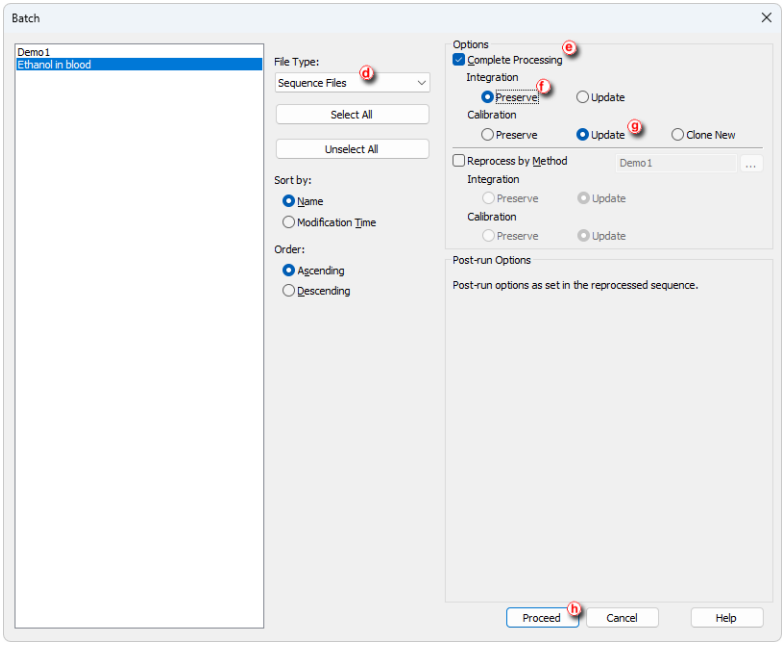
Note: To print or export the data the chromatogram has to be opened in the *Chromatogram* window - this is achieved by checkbox in the *Open* ⓑ column on a given row.



4. Open the *Batch* dialog by using *Analysis - Batch* in the *Instrument* window.
5. Switch *File Type* to *Sequence Files* ⓓ .
6. Select the Sequence you wish to reprocess.
7. Check the *Complete Processing* ⓔ checkbox.
8. To preserve manually updated integration (this mainly considers small individual adjustments where optimized parameters weren't satisfactory) select the *Preserve* ⓕ in the *Integration*part of *Options* section.

9. To perform recalibration based on updated integration select *Update* ⓖ in the *Calibration* part of *Options* section.
10. *Proceed* ⓗ with the batch processing.

The recalibration will be performed and post-run options defined in the sequence will be performed.



Caution: The operations during Batch reprocessing are done row after row, injection after injection. In some situations it is necessary to perform the Complete Processing in two steps - first just the recalibrations, second the post-run actions (either using the Complete Processing again with the Integration a Calibration settings in the Options section to Preserve, or through running the post-process on selected chromatograms only through procedure described in Performing Post-run Options from Batch dialog section). For example, if the sequence is using calibration bracketing the unknowns are measured before second standards set and if the unknowns were reported during the recalibration step, the responses from the second standards set would be missing in the report.

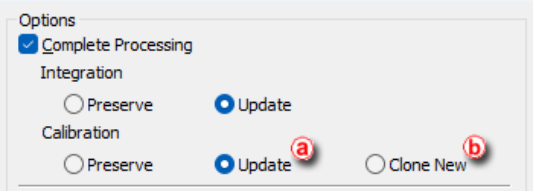
11.2 Reprocessing whole sequence while using calibration cloning

If you are using any kind of the calibration cloning in the sequence the reprocessing whole sequence is similar to regular reprocessing described in the previous topic.

Please refer to the Calibrating using clone on first recalibration, Compensating for response drift using bracketing or Improving quantification with the standard addition method topics to learn more about Calibration Cloning in Clarity.

The difference from the standard Reprocessing procedure described in Reprocessing whole sequence topic is shown below.

- In the *Batch* dialog you have additional option for calibration behavior, the meanings of options are:
  - If you select Update ⓐ in Calibration part of Options section the calibration(s) that are currently linked to measured chromatogram(s) will be recalibrated (new cloning is NOT performed).
  - If you select Clone New ⓑ in Calibration part of Options section new calibration(s) will be created as if the sequence was run again (new clone (s) are created and linked to chromatograms).



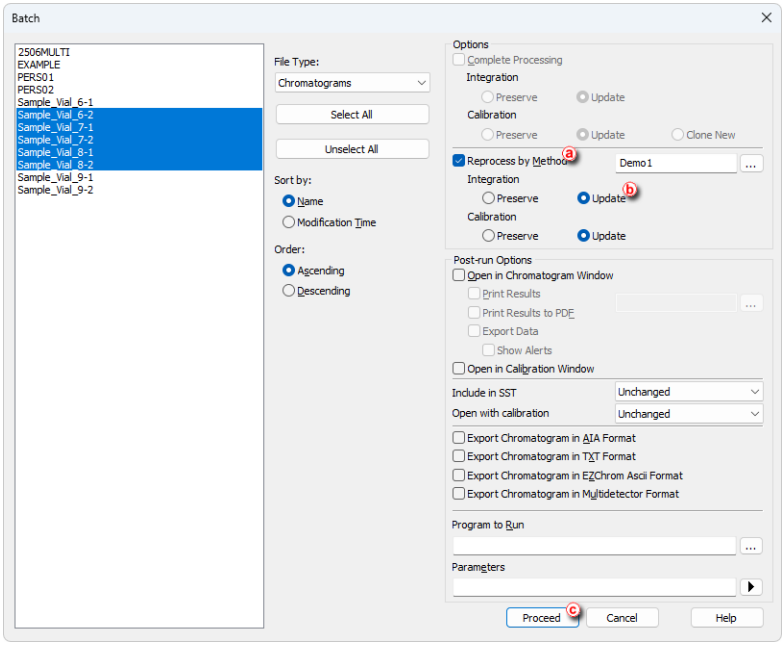
11.3 Reprocessing by selected method

Reprocessing by method is suitable for applying Integration parameters to previously measured chromatograms after these parameters were saved to the method by Save Method as a Template. You can also changed the link to the calibration file without the calibration being reprocessed.

Note: If the Sequence file is selected to be reprocessed by method, all currently linked chromatograms will be reprocessed. No recalibration is carried out, when *Calibration - Update* is selected only links to calibration are changed without any changes to the calibration file itself.

1. Prepare your method with desired integration and linked calibration.
2. Open *Batch* dialog by menu *Analysis - Batch...* from the Instrument window.
3. Select chromatograms you want to reprocess (Alternatively, select sequence(s), depending on your *File Type*).
4. Select *Reprocess by Method* ⓐ and define your created method.
5. Select *Update* ⓑ Integration in case you want to change integration parameters as set in the defined method.
6. Click on Proceed ⓒ .

Note: *Reprocess by Method* can be combined with *Post-run Options* if you are sure that changes in chromatograms do not have to be reviewed before exporting/printing.



Now your chromatograms are reprocessed, with linked calibration file and amended integration parameters from the used method.

11.4 Performing Post-run Options from Batch dialog

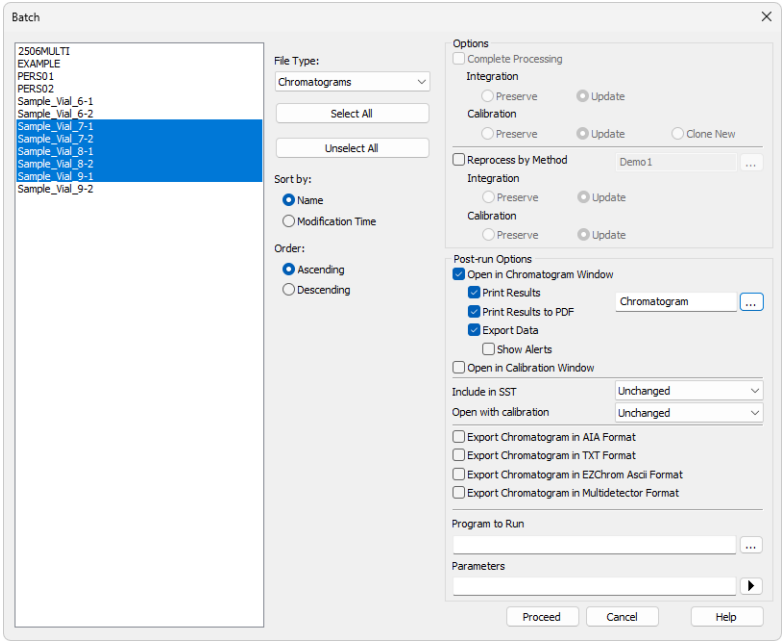
This procedure is useful if you need to *Print* or *Export* more chromatograms at once, e.g. after all of them were reviewed and signed.

1. Navigate to *Batch* dialog by clicking *Analysis - Batch* in *Instrument* window.
2. Select chromatogram(s)/sequence(s) that you want to print reports for (when sequence file is selected, all chromatograms that are currently linked in it will be reported). Which files are displayed is based on *File Type* drop-down menu.
3. Select *Open in Chromatogram Window* to be able to select *Print Results* and/or *Print Results to PDF* and/or the *Export Data* (or select any other option).
4. Select report style you would like to use by clicking ... button.
5. (Optional) change *Open with Calibration* to *Stored*, this will ensure that data will be printed in the state they were saved in last time.

   Note: By default chromatograms are opened with *Linked* calibration. If the calibration was changed after saving chromatograms the results might be influenced.

6. Click *Proceed*.

Note: It is also possible to process data before printing them by using *Complete Processing* or *Reprocess by Method* options. When *Complete Processing* is selected, the post-run options are governed by settings in reprocessed sequence. For more info see chapter regarding Batch dialog for more info.



12 Results and Calculations

Advanced topics describing how to use *User Columns* to calculate custom results, etc.

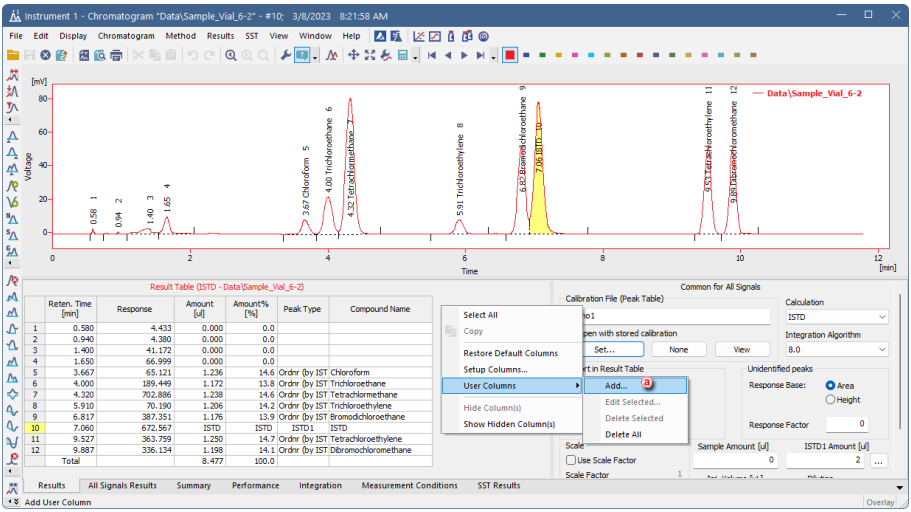
12.1 User Columns

This article describes how to append a new column with user-defined calculation to the *Chromatogram - Result Table*. For more details about User Columns refer to **Reference Guide Manual**.

Note that majority of calculations require chromatogram to be calibrated. Without it the necessary values are not available.

Caution: *User Columns* are stored in .DSK files. If the station is used by more users and *User Columns* are needed it is recommended to set shared .DSK file as described in chapter "Sharing settings among users".

1. Open a chromatogram you want to work with and switch to *Results* tab.
2. Right click on the *Result Table* and select *User Columns - Add...* ⓐ , the *Add User Column dialog* will be opened.

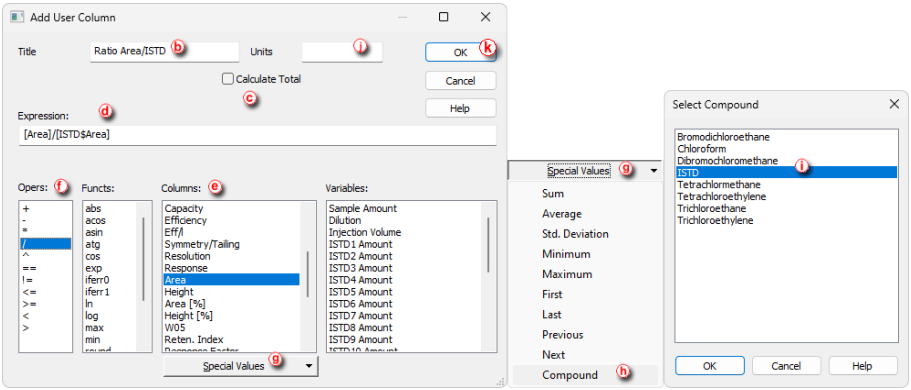


3. Fill in the *Title* ⓑ of the new column. In our case *Ratio Area/ISTD*.
4. Check/Uncheck *Calculate Total* ⓒ (depends on whether sum of calculated values has a meaning).
5. Fill in *Expression* ⓓ line , which presents the user's defined calculation. In our case:

- In *Columns:* ⓔ list double-click *Area*.
- In *Opers:* ⓕ list double-click */*.
- In *Columns:*list select *Area*, then click on *Special Values* ⓖ , select *Compound* ⓗ , choose *ISTD* ⓘ and click *OK*.

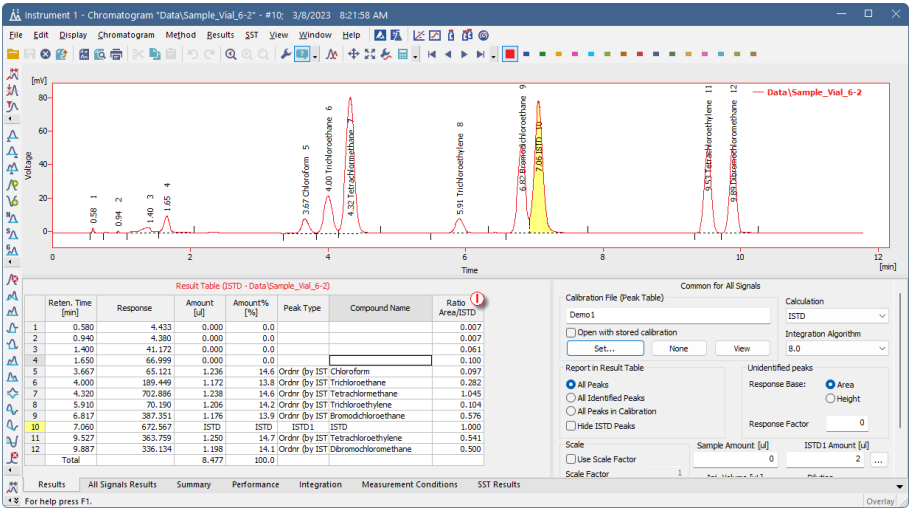
6. Fill in appropriate *Units* ⓙ based on the formula.
7. Click *OK* ⓚ in the *Add User Column* dialog.

Note: It is possible to fill *Expression* by typing if you know the correct syntax.



8. New *User Column* is added to the Result Table ⓛ .

Note: You can edit existing *User Columns* by right-clicking into them and selecting *User Columns - Edit Selected...*.

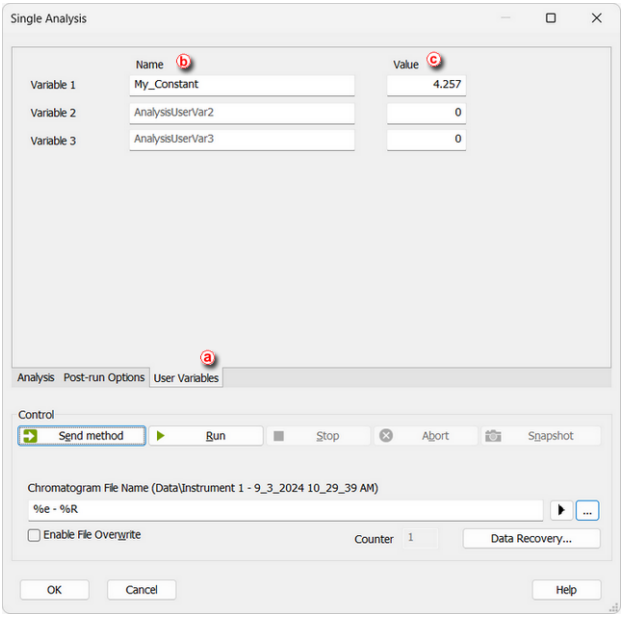


12.2 User Variables

This article describes how to set *Analysis* and *Method User Variables* which can be subsequently used in *User Columns* calculations. *Analysis User Variables* can be defined in *Single Analysis* or *Sequence* window. *Method User Variables* can be defined in *Method Setup* window.

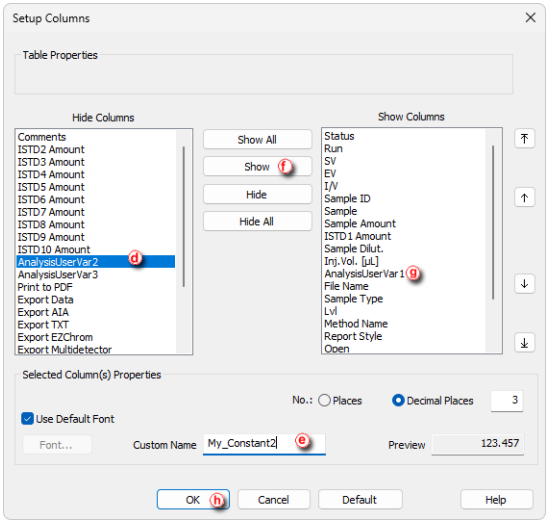
A) Setting of Analysis User Variables in Single Analysis window

1. In *Single Analysis* dialog navigate to the *User Variables* tab ⓐ .
2. Define *Name* of the variable ⓑ . If the field is left empty, default name *AnalysisUserVar1-AnalysisUserVar3* will be used.
3. Define numerical *Value* of the variable ⓒ .

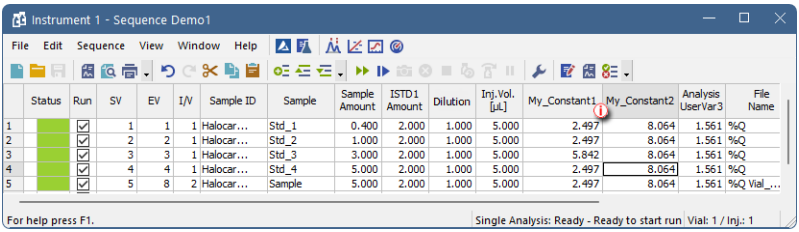


B) Setting of Analysis User Variables in Sequence window

1. In *Sequence* window the *AnalysisUserVar1 - AnalysisUserVar3* columns are hidden by default.
2. To display them right-click on the *Seqeunce Table* and use *Setup Columns...* command.
3. Select the variable in the *Hide Columns list* ⓓ , fill its name ⓔ and click *Show* ⓕ (item will be move to the *Show Columns* list ⓖ).
4. Repeat the previous step if more variables are needed then click *OK* ⓗ .

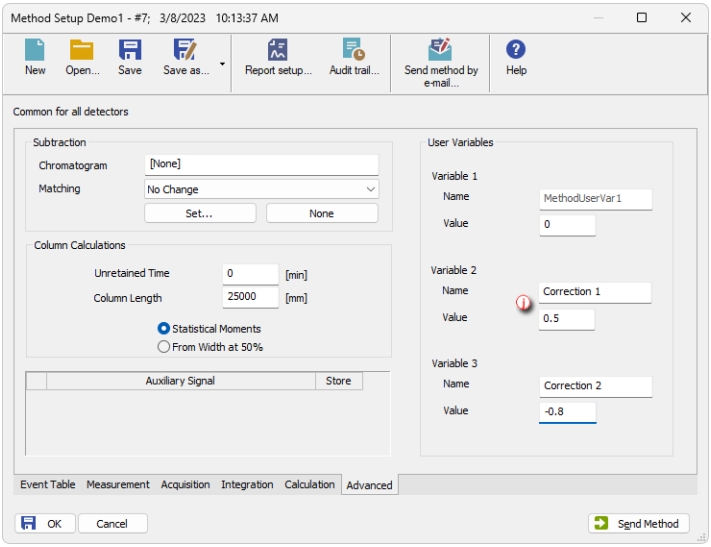


5. Defined *Custom Name* of the variable is used directly in the column header ⓘ . Fill in the values for each row (different values can be used).



C) Setting of Method User Variables in Method Setup window

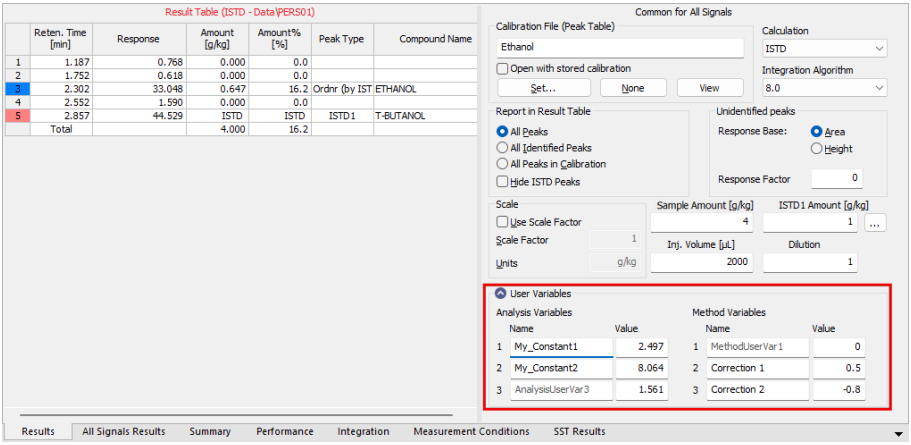
1. In the *Method Setup* dialog navigate to *Advanced* tab
2. Define *Name*, numerical and *Value* of the variables that should be used ⓘ . Default name *MethodUserVar1-MethodUserVar3* is used when the *Name* is empty.



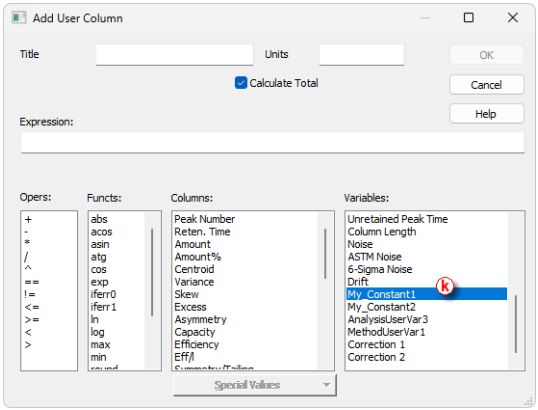
D) Setting of User Columns with User Variables

Analysis and *Method User Variables* are also editable directly from *Chromatogram* window on *Results* tab in *User Variables* section (it is collapsed by default and must be expanded by clicking the arrow symbol).

Variables can be modified in the same manner as in the previous cases.



Note: To use variables in custom calculations add *User Column* as described in chapter "User Columns" and while formulating the *Expression* select the desired variable from *Variables* list ⓚ .



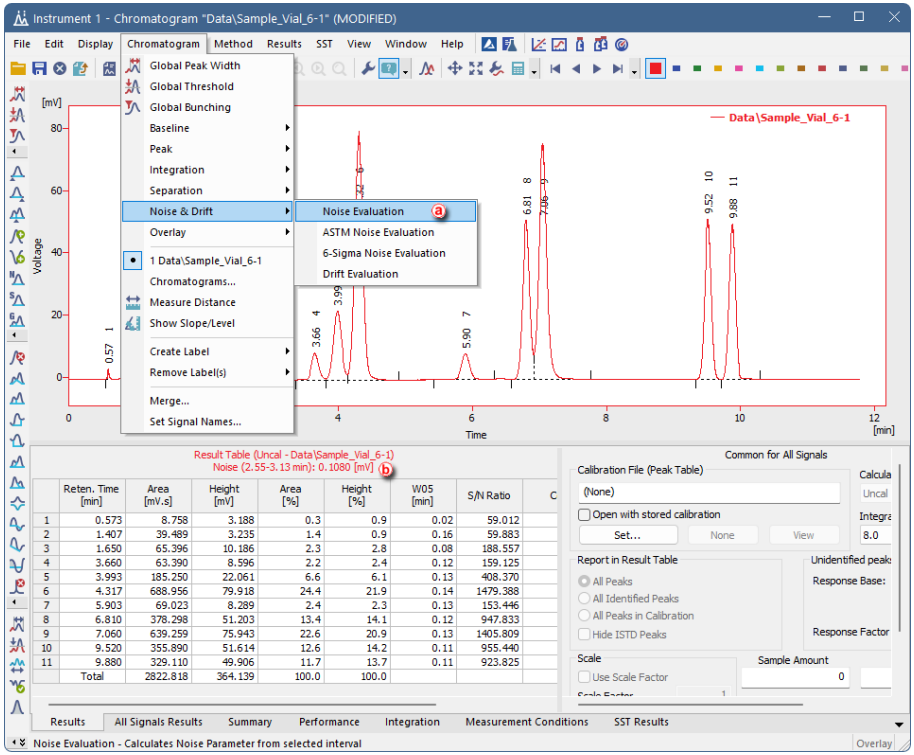
12.3 Signal to Noise Ratio Calculation

This article describes how to calculate Signal to Noise Ratio using *User Columns* calculations with *Variables*.

12.3.1 Noise Parameter Evaluation

At first *Noise* value has to be evaluated. This value is subsequently used to calculate the *Signal to Noise Ratio*.

1. Open measured chromatogram in the *Chromatogram* window
2. Use *Chromatogram - Noise & Drift - Noise Evaluation* ⓐ and select the interval for noise calculation. The same result can be obtained from the *Integration Table* after selecting the *Evaluation - Noise* operation and inputting the desired interval manually.
3. The value of the evaluated Noise Parameter is shown in the *Result Table* header ⓑ .
4. For the same chromatogram such value is stored as a *Noise* variable in the *Edit User Columns - Variables* ⓔ .



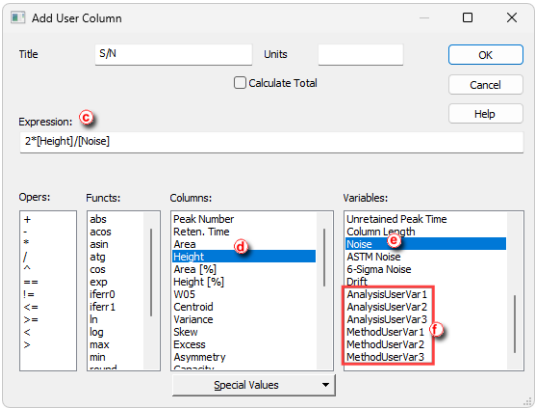
12.3.2 Calculating Signal to Noise Ratio

Signal to Noise Ratio is important parameter used for method validation. Most commonly used generic formula for Signal to Noise = 2*Peak Height/Noise.

For such calculation, two possible approaches exist:

- The *Noise* is determined from the same chromatogram within area with no peaks. The *Noise* variable ⓔ can be used directly in the formula entered in the *Expression* ⓒ edit box. In that case the resulting formula will be for example 2*[Height]/ [Noise], where both parameters are determined from the same chromatogram.
- The *Noise* is determined from other chromatograms (e.g., by measuring blanks and evaluating the *Noise* in the area of expected peak). In the *Edit User Column* dialog in the *Expression* ⓒ edit box use the [Height] ⓓ from the Columns section for peak height and enter the calculated *Noise* value as a constant. The resulting formula will be then e.g. 2*[Height]/0.1080, where the number 0.1080 is the calculated *Noise* parameter. Alternatively, the calculated *Noise* parameter could be stored as a *Method User Variable* or as an *Analysis User Variable* ⓕ to

simplify changes of the value - this variable can be then used instead of entering the numerical value in the *Expression* edit box.



Note: In the *Expression* edit box, variables are treated as numbers, therefore operators and numbers can be used to modify the formula. The resulting formula can be e. g. 2* [Height]/ [Noise] or 2* [Height]/ [UserVariableNoise] (where the [UserVariableNoise] represents user variable to which the Noise value determined from chromatogram blank is stored) or 2*[Height]/0.1080 (where the 0.1080 represents the actual Noise value determined from chromatogram blank).

Note: Setting the *Analysis User Variable* or the *Method User Variable* is described in the section **User Variables on pg. 156**.

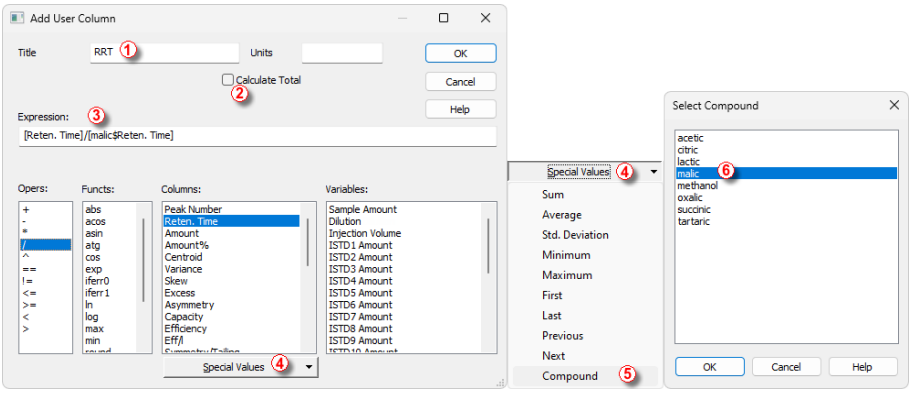
12.4 How to calculate Relative Retention Time

This chapter describes how to calculate Relative Retention Time (RRT). In Clarity, there are basically two ways how to achieve that. In the first one, there is peak in the chromatogram that you want to use for the calculation. In the second approach, you fill in the time for an Unretained Peak and then use it for the calculations.

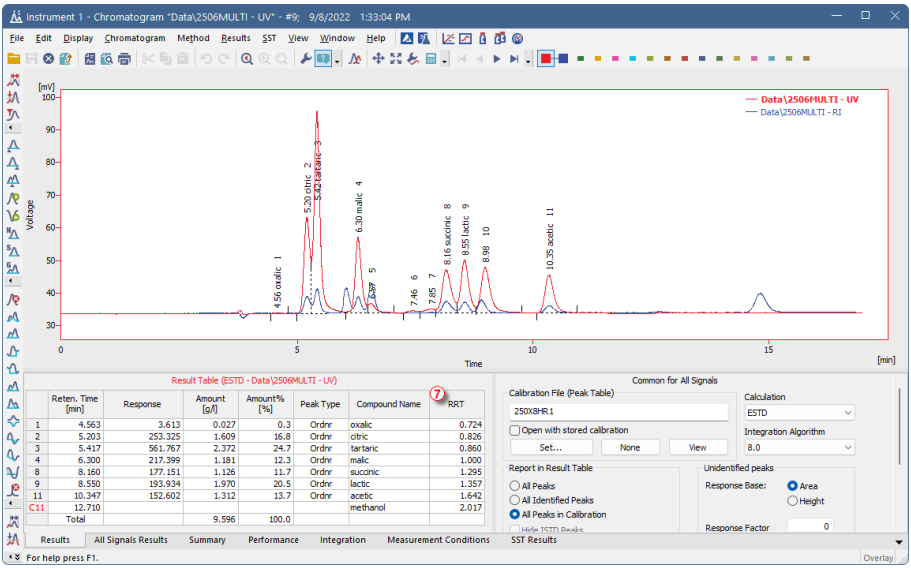
12.4.1 Relative Retention Time calculation based on an existing peak

1. Open a chromatogram you want to work with and switch to *Results* tab.
2. Add a *User Column* as described in chapter "User Columns".
3. Fill the *Title* for the new column - e.g., *RRT* ① .
4. Uncheck *Calculate Total* ② .
5. Enter "*[Reten. Time]/[malic$Reten. Time]*" formula to the *Expression* field ③ , where "malic" represents your compound which should be used for calculation of RRT. You can either use items from the *Columns:* list or type them manually.

Note: To insert *[malic$Reten. Time]* select *Reten. Time* in *Columns:* list, click *Special Values* ④ , in the drop-down list select *Compound* ⑤ , and in the following dialog, select the compound ⑥ you want to use for calculation of RRT (the list is based on the used calibration file).



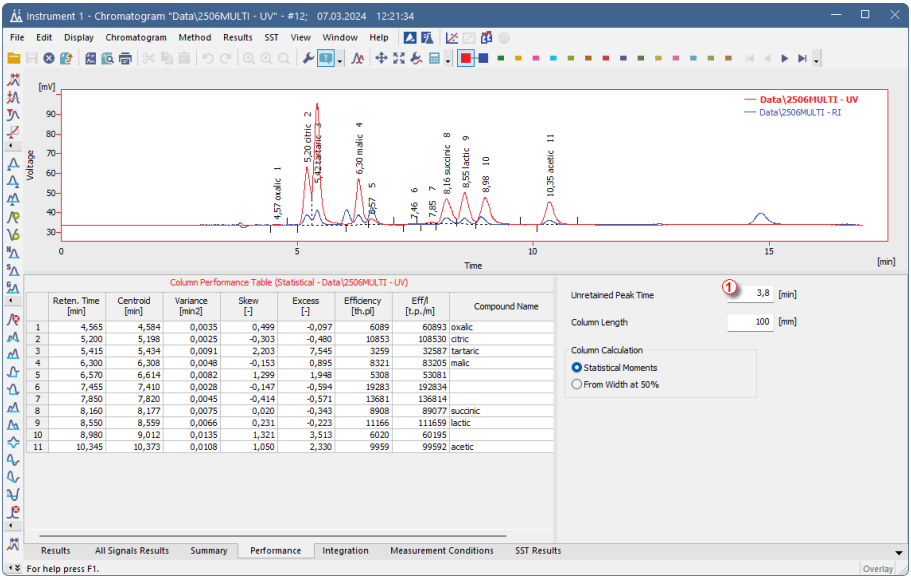
6. Close the *Add User Column* dialog using *OK*
7. A new *RRT* column ⑦ is displayed in the *Result Table*.



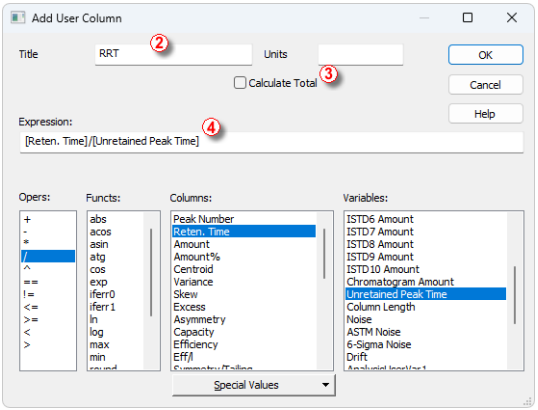
Note: You can do a quick check that the calculation is correct: look at the *malic* compound, the RRT shoud be *1*.

12.4.2 Relative Retention Time based on the Unretained Peak variable

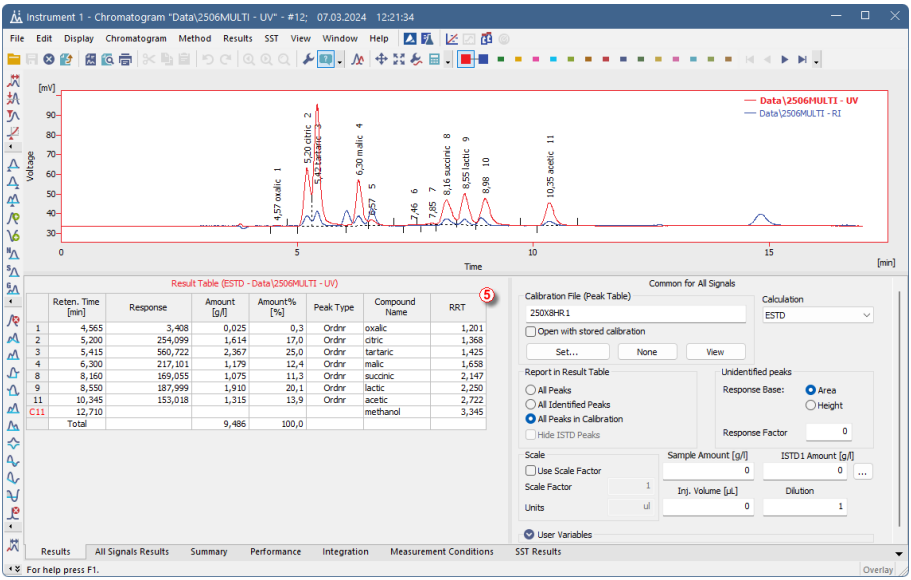
1. Open the chromatogram you want to work with and switch to the *Performance* tab.
2. Fill in the *Unretained Peak Time* as you need ① .



3. Go to the *Results* tab.
4. Add a *User Column* as described in chapter "User Columns".
5. Fill the *Title* for the new column - e.g., *RRT* ② .
6. Uncheck *Calculate Total* ③ .
7. Enter "*[Reten. Time]/[Unretained Peak Time]*" formula to the *Expression* field ④ . You can either use items from the *Columns:* and *Variables:* lists or type them manually.



8. Close the *Add User Column* dialog using *OK*.
9. A new *RRT* column ⑤ is displayed in the *Result Table*.

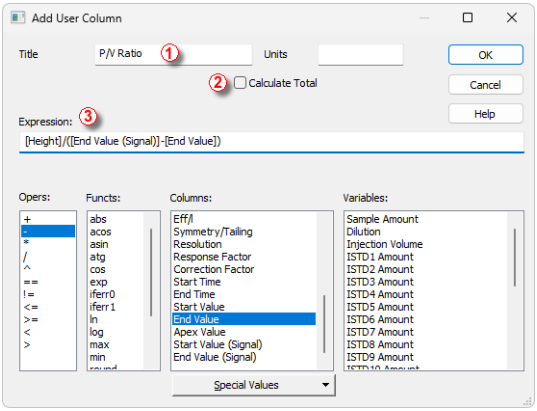


12.5 How to calculate Peak to Valley Ratio

This chapter describes how to calculate Peak to Valley, which is a ratio of signal height in peak apex and signal height in the end of peak. This ratio is used for e.g., impurity determination.

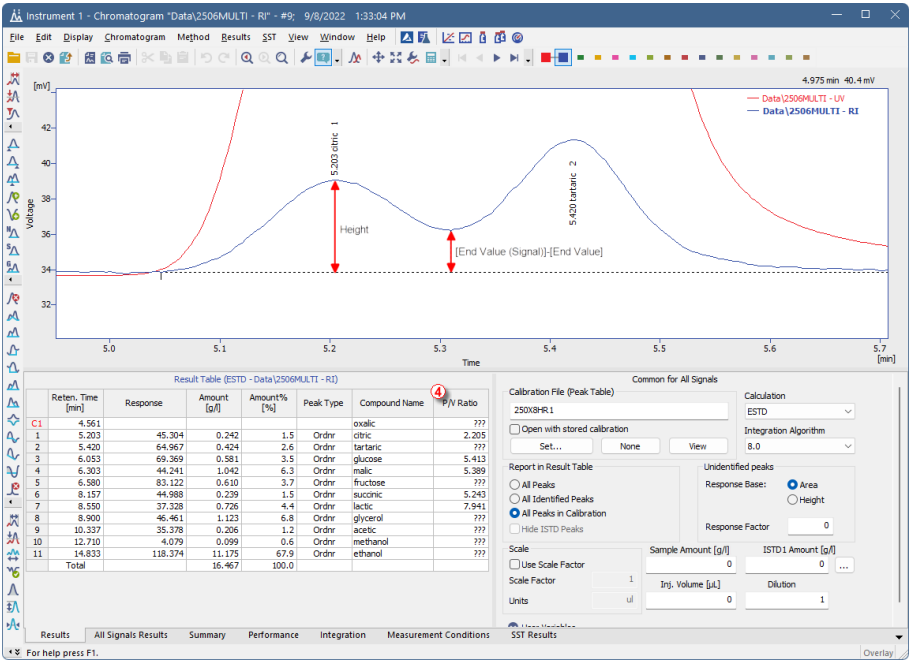
1. Open a chromatogram you want to work with and switch to *Results* tab.
2. Add a *User Column* as described in chapter "User Columns".
3. Fill the *Title* for the new column - e.g. *P/V Ratio* ① .

4. Uncheck *Calculate Total* ② .
5. Enter "*[Height]/([End Value (Signal)]-[End Value])*" formula to the *Expression* field ③ . You can either use items from *Columns:* list or type it manually.
6. Close the dialog by clicking *OK*.



7. New *P/V Ratio* column ④ is displayed in the *Result Table*.

Note: Value is only valid for peaks, where peak end is not on the baseline.



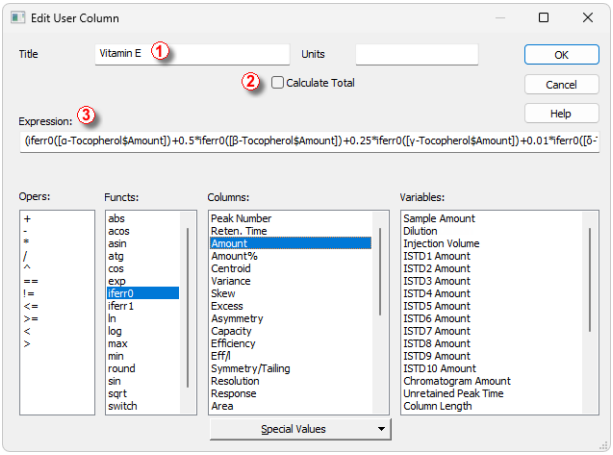
12.6 How to handle not-found compounds in your calculations

If any compound is missing from a chromatogram, its amount is not calculated. In any equations within *User Columns*, where this amount would be used, the calculations would produce ??? (invalid result). In such cases, the *iferr0* function can replace the missing value with 0 (analogically, the *iferr1* function replaces the missing value with 1). This functionality can be used in situations, when a substance is present in multiple chromatogram peaks, possibly even in different ratios. *User Columns* can be used to determine its total content. The *Expression* (equation) would then contain the Amounts of compounds in the chromatogram. However, some of the compounds may not be present in the evaluated chromatogram. The following case scenario shows how the *iferr0* function can be used. The goal is to calculate the content of Vitamin E in different Tocopherols.

1. Open a chromatogram you want to work with and switch to *Results* tab.
2. Add a *User Column* as described in chapter "User Columns".
3. Fill the *Title* for the new column - e.g. *Vitamin E* ① .
4. Uncheck *Calculate Total* ② .
5. Enter the formula for calculating the vitamin E content, e.g., "*([α-Tocopherol$Amount]+0.5* [β-Tocopherol$Amount]+0.25* [γ-Tocopherol$Amount]+0.01*[δ-Tocopherol$Amount])/10*" to the *Expression* field.

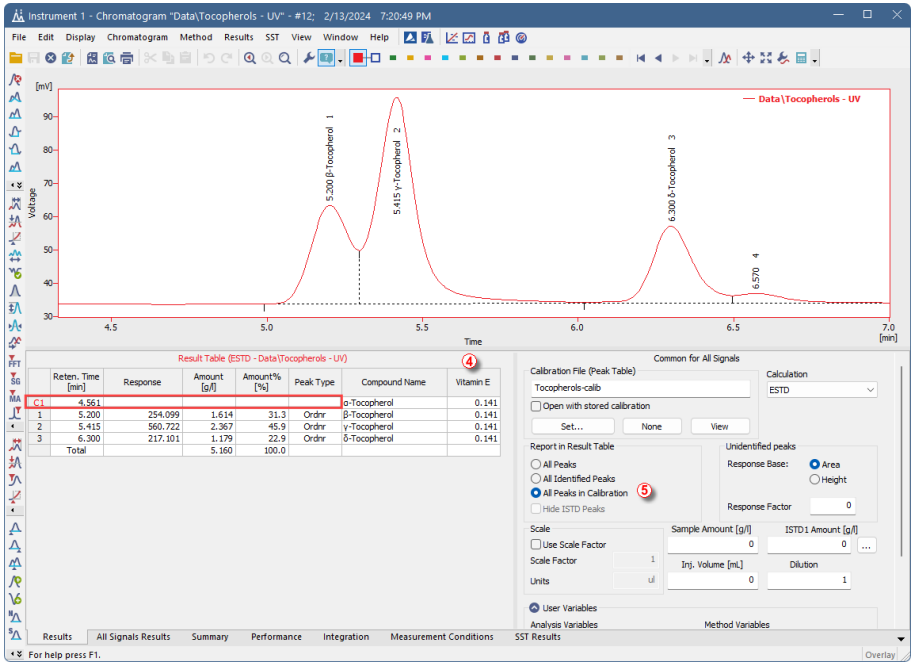
You can either use items from the *Columns:* list with *Special Values* or type it manually.

6. Apply the *iferr0* function on the items that may be missing from the result table. The resulting function will look like the following: *(iferr0 ([α-Tocopherol$Amount])+0.5*iferr0 ([β- Tocopherol$Amount])+0.25*iferr0 ([γ-Tocopherol$Amount])+0.01*iferr0([δ-Tocopherol$Amount]))/10* ③ .
7. Close the dialog by clicking *OK*.



8. The new *Vitamin E* column ④ is displayed in the *Result Table*.
9. In the case that any of the compounds is not found in the chromatogram (such as here, in the case of α-Tocopherol), the Amount is not calculated. The *iferr0* function replaces the not-found Amount with zero in further calculations.

Note that the *All Peaks in Calibration* ⑤ option is selected. Otherwise, the missing compound would not be present in the *Result Table*, and the calculation would not be possible.



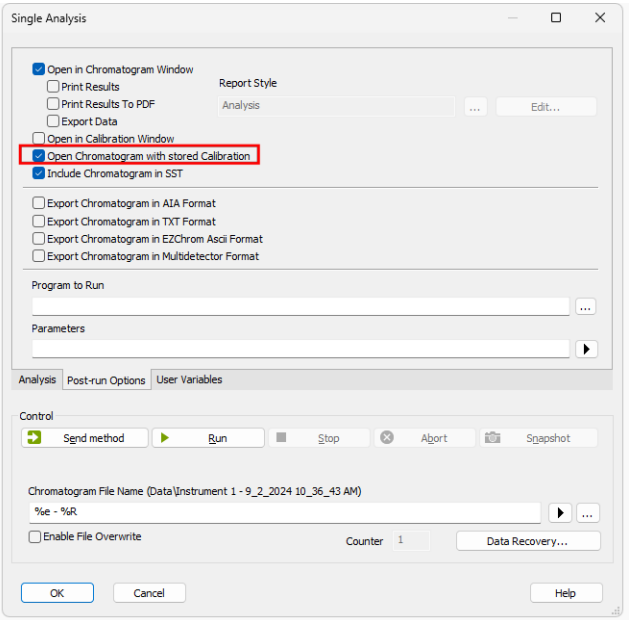
12.7 How to display older results when linked calibration is modified

Clarity does not store any results in the chromatogram, the result table is always calculated from the actual state of the calibration file referenced in the *Calibration Table (Peak Table)*, i.e. *Linked* calibration. Any changes in this calibration will be immediately reflected in the displayed results. Each time a chromatogram is saved the current state of the linked calibration is stored (i.e. *Stored* calibration) in the chromatogram history (just values needed to calculate the results, not a complete calibration). Chromatogram opened with a version from history (i.e. opened with *Stored* calibration) will display results as they were at that time.

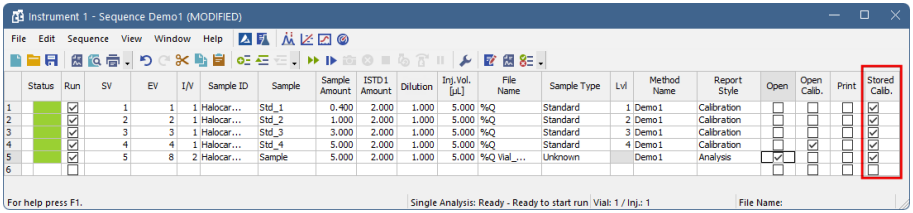
In case the calibration file is reused for some time, opening the chromatogram with linked calibration will show changed results due to changes in the linked calibration. To avoid this, two approaches are possible:

1. Make a copy of the calibration file so each series of measured chromatograms will be linked to a separate calibration file. This has advantage in case some amendments to the calibration will be necessary later, as the amendments will affect only the related chromatograms. Such procedure could be automated from sequence. For more information regarding this procedure, see the chapter **"Calibrating using clone on first recalibration"** on pg. **112**..

2. Using the *Open with stored calibration* option. Such option is accessible from multiple dialogs, depending on whether Single Analysis or Sequence is measured (automated approach) or this option can be selected upon opening the chromatogram.
    - In the *Single Analysis* dialog - *Post-run Options* tab, select the *Open Chromatogram with stored Calibration* option.



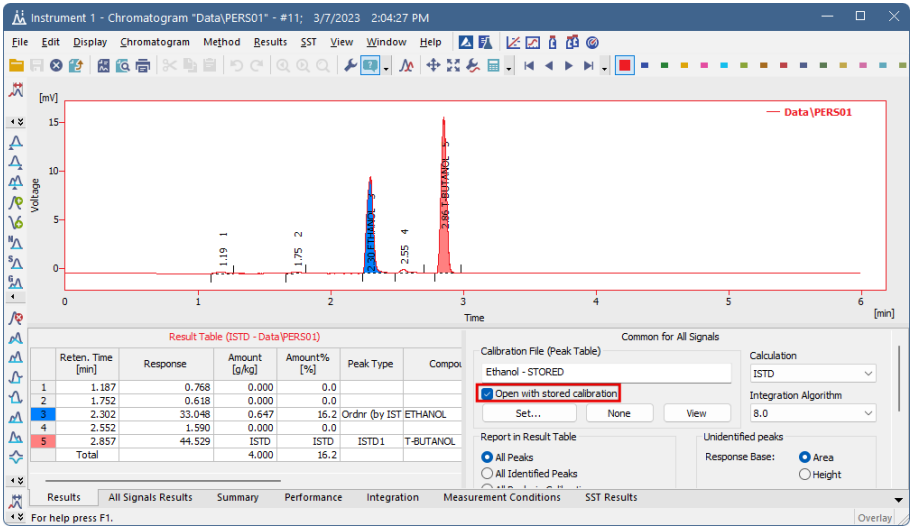
    - In the *Sequence* window select checkbox in the *Stored Calib.* column. By default, *Stored Calib.* column is hidden. To show it, right mouse click in the sequence table and choose *Setup Columns...*. From the *Setup Columns* dialog, choose *Stored Calib.* from the left list and click on the *Show* button - it will be added to the show list. Once you click the *OK* button, you will return to the *Sequence* window and the new *Stored Calib.* column will be added.



    - In the *Chromatogram* window select *Open with stored calibration* option. This will open the chromatogram with the most recent point

from history and show the results according to the stored calibration. Any changes in the linked calibration will not affect those results. To open the chromatogram with the stored calibration this way it is necessary to re- open the chromatogram using the *Open Chromatogram* dialog - re-opening the *Chromatogram* window is not sufficient.

Note: This setting is only applied and saved to the currently opened chromatogram. It will not be transferred to the next (different) opened chromatogram.



12.8 Calculating percentage content of a compound in a solid sample

This is a standard procedure used across various chromatography applications - a known amount of a sample is dissolved in a known volume of a solvent and the goal is to determine the percentage content of the compound in the sample.

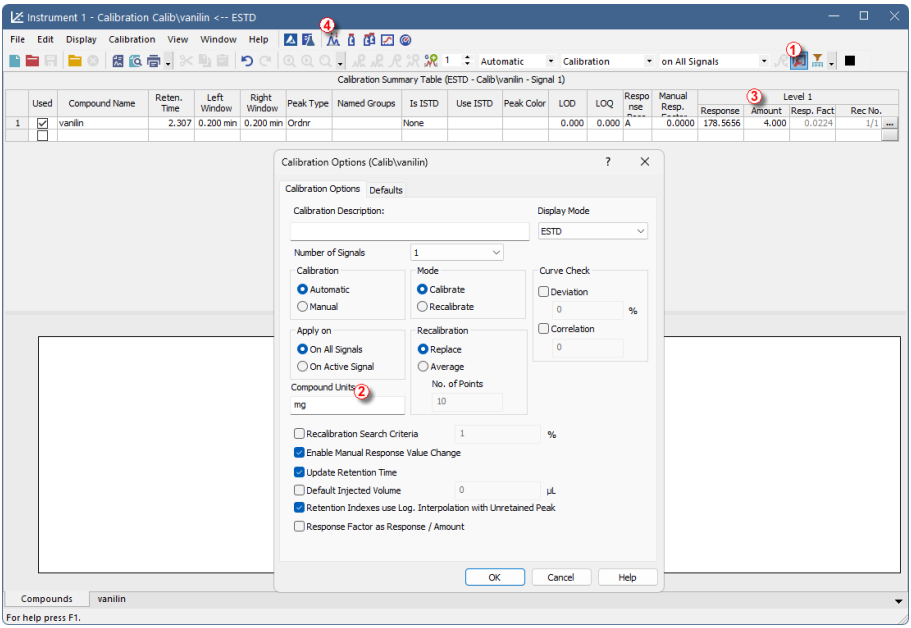
1. Open your calibration/create a new one in the *Calibration* window.
2. Click the icon to open *Calibration Options* dialog ① .
3. Specify used unit for the amount in *Compound Units* field ② . Confirm changes by clicking *OK* button.

Note: Fill the unit used for the total amount of sample. In our specific case sample was weighted and *mg* is used. Set units are used in the *Chromatogram* window for further calculations.

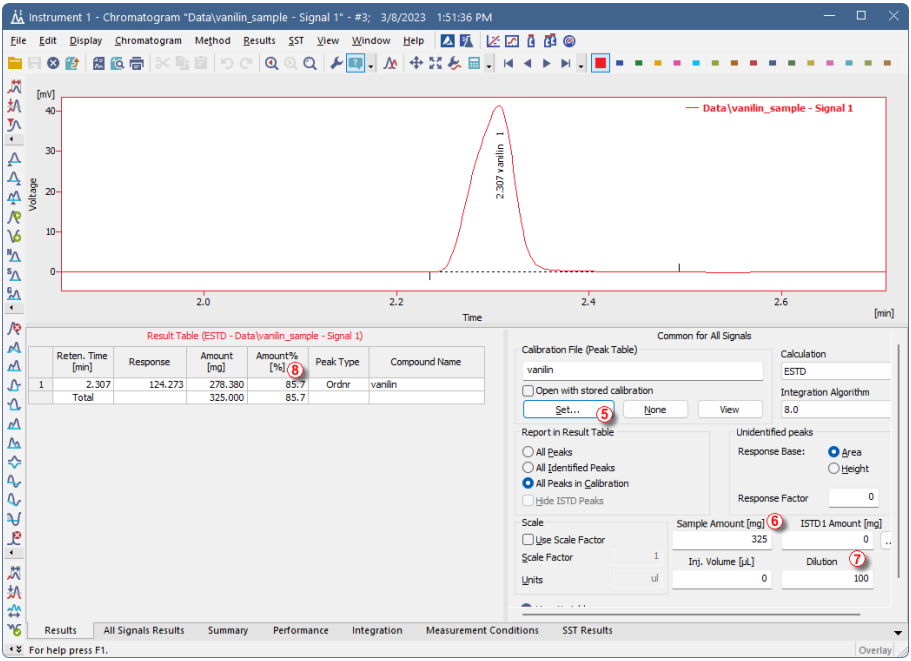
4. Fill corresponding *Amount* for each compound as concentration ③ .

Note: That means amount divided by the volume of solvent used to prepare the standard solution. In our example *400 mg* of **vanilin** was dissolved in *100 ml*, thus the *Response* from the standard chromatogram corresponds to *4 mg/ml* which is the value entered in the *Amount* field in the calibration.

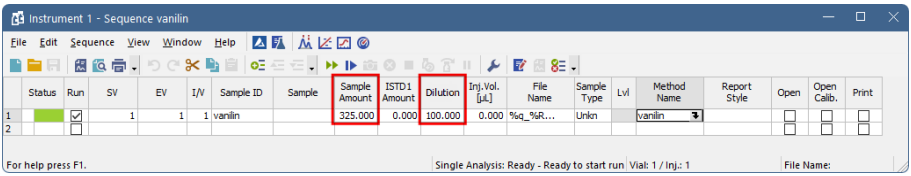
5. Save the calibration and open *Chromatogram* window ④ .



6. Open chromatogram(s), assign each chromatogram prepared calibration using the *Set...* button ⑤ .
7. Fill the amount of the sample that had been used ⑥ . *Sample Amount* refers to the mass of the sample used. Units are automatically copied from the *Calibration Options* (see step 3). The entered amount replaces the *Total* value in the *Amount* column of the *Result Table*. In our example: *325 mg* of sample had been used.
8. Fill the dilution that had been used ⑦ . *Dilution* refers to the solvent volume that has been used to dilute the sample. Dilution multiplies the values in the *Amount* column of the *Result Table*. In our example: *325 mg* of sample had been diluted by *100 ml* of solvent.
9. Column *Amount%* in the *Result Table* now displays the percentage amount of the compound in the sample ⑧ .

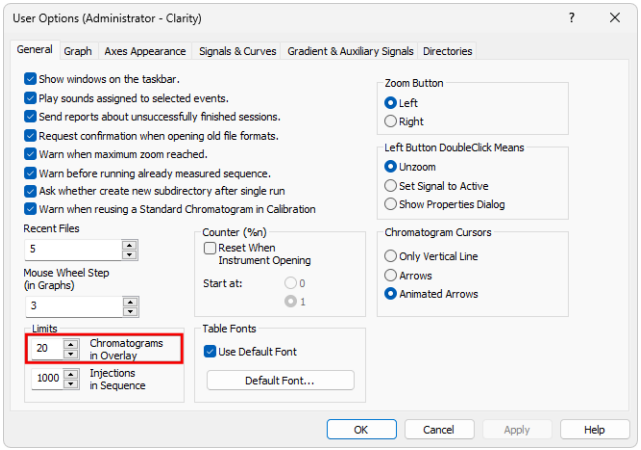


Note: It is possible to automatize this process. Calibration can be linked to the used method so it is automatically linked. *Sample Amount* and *Dilution* can be pre-filled in *Single Analysis* or *Sequence* windows.



12.9 Comparing the results from several chromatograms

The default maximum number of chromatograms in Overlay is set to 20. In case summary report should include more chromatograms, this limit can be changed in the User Options window, which can be invoked from the *Instrument window* by using *Setting - User Options...*.

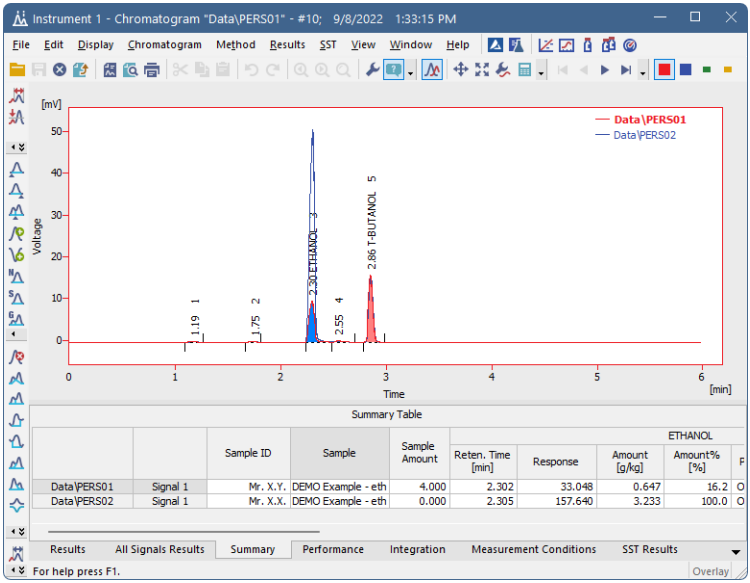


1. Open the chromatograms using *File - Open Chromatogram....* In *Open Chromatogram* dialog select desired chromatograms and click *Open in Overlay*.

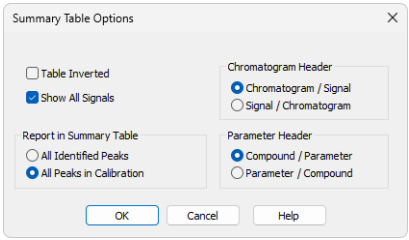
   Note: You can also use *File - Open Chromatograms From Sequence...* command which opens all chromatograms from sequence including Standards.

2. Click on the *Summary* tab in the lower part of the window to display the *Summary Table*. In the rows you can see chromatograms and signals with measured values and in the columns there are identified peaks from all calibrated chromatograms.

   Caution: *Summary Table* is based on calibration meaning only calibrated peaks will be present in it.



3. Right click on the *Summary Table*, if you want to change the visualization of the table or add a custom column, etc.
4. To see all signals, select the *Show All Signals* checkbox in the *Summary Table Options* dialog accessible from the pop-up menu of the *Summary Table*. By default, only signals containing calibrated peaks are visible in the *Summary Table*.



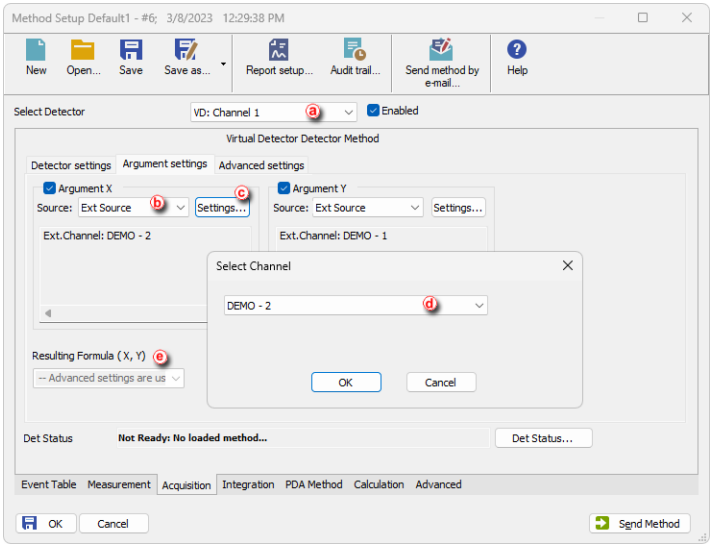
Note: It is also possible to compare parameters from different chromatograms and check if they fall within set limits by using the SST Extension.

12.10 Confirming the identity of a compound by using the signal ratio

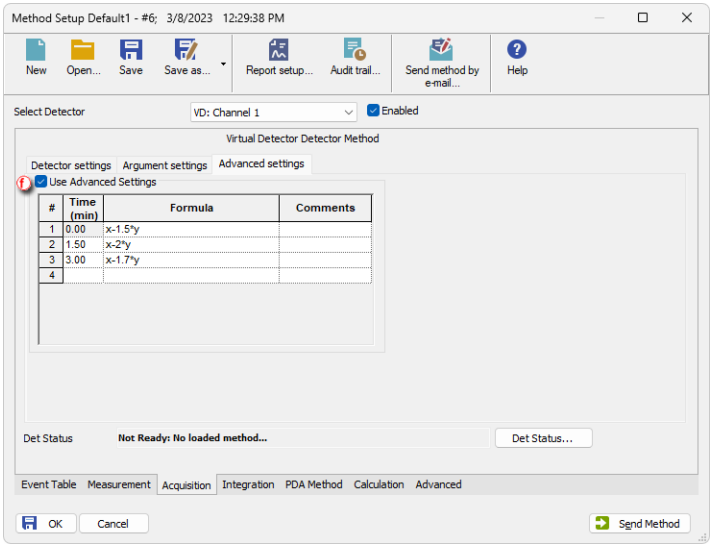
The identity of a compound can be confirmed by using a dual wavelength detector in conjunction with the Virtual Detector and checking if the signals ratio is constant with the following procedure. Prerequisite to this is a know signal ratio for used wavelengths. With correct comparison formula the Virtual Detector signal should

result in flat line when the peak is pure compound, impurities with different signal ratio would be represented as response change on the Virtual Detector signal.

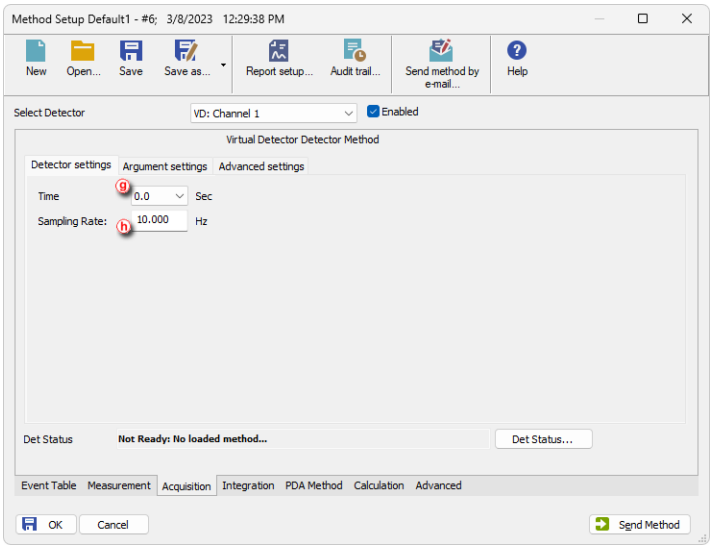
1. Add the Virtual Detector as well as your dual wavelength detector to the instrument, if not already present, based on chapter *Adding a new device*.
2. Open the Method Setup dialog and navigate to *Acquisition* tab.
3. Select *VD: Channel 1* in the *Select Detector* drop-down list ⓐ .
4. On the *Argument settings* tab, tick the *Argument X* checkbox, select an *Ext. Source* ⓑ , then click on the *Settings* button ⓒ , select the appropriate detector *Channel* ⓓ and click *OK* .
5. Repeat the same steps for *Argument Y* and select the second channel from the detector.
6. If want to use the same signal ratio for entire analysis you can fill in the Resulting Formula field ⓔ with the proper formula. If you need multiple formulas for different times skip this step and continue with the next one.



7. To set multiple formulas for different time intervals navigate to the *Advanced settings*, check the *Use Advanced Settings* ⓕ checkbox and fill the time table as needed.



8. On the *Detector settings* tab, set the *Time* to 0 ⓖ to avoid distortion and fill *Sampling Rate* ⓗ equal to the actual detector sample rate.



Method prepared this way can be used to check compound identity as mentioned in the beginning of this chapter.

13 Data Reports

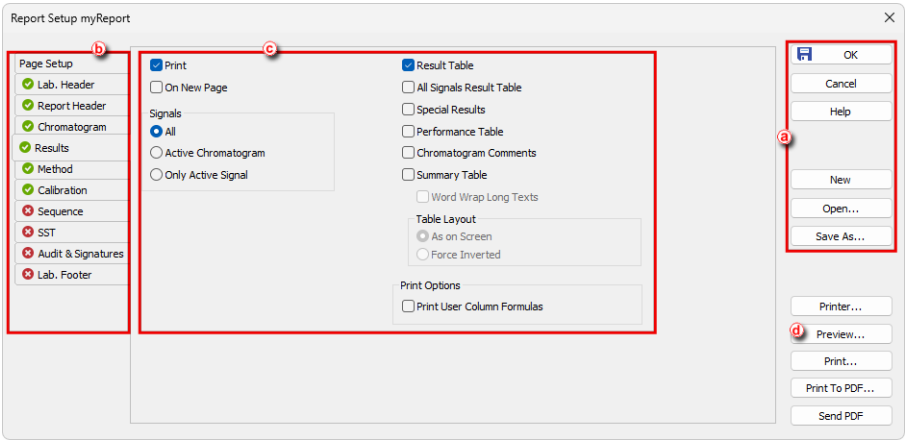
Following chapters describe how to create a report, adjust it and print.

13.1 Setting up a report style for printing

It is possible to select what information and how you want to have printed in the report. You can create different report styles and store them in different *.STY files.

To see an example on how to set up a style to obtain a specific layout see chapter *Creating a report (example)*.

1. From the *Instrument, Calibration, Chromatogram* or *Sequence* windows, select *File - Report Setup*. From the *Method Setup* window click the *Report Setup* button.
2. Click the *New* button if you wish to create a new report style or click the *Open* button ⓐ to open existing report style. Name of currently opened style is included in the window header.
3. Select the tab corresponding to the section you wish to modify ⓑ .
4. Click and drag the tabs to a new position if you wish to change the order in which they will be printed in the report. Tabs can also be moved via context menu which is invoked after right-clicking on them. The first two (*Page Setup, Lab. Header*) and last two (*Audit & Signatures, Lab. Footer*) tabs have fixed position.
5. Select options you would like to include in that section. ⓒ
6. Click *Preview* ⓓ to see the result preview and repeat steps 3.-5. if you wish to modify anything.
7. Click *Save As* to save the report style under a new name or *OK* to accept the changes to the current style. ⓐ



13.2 Printing or previewing a report

The report may include information about methods, calibrations, chromatograms etc. It is possible to setup what information you would like to include in the report as explained in *Setting up a report style*.

Caution: While setting reports it is necessary to pay attention to several crucial settings bellow:

- The information on the report will vary depending on which window we open it from, even if we use the same report style.
  For example, the Chromatogram tab in the Chromatogram Report Setup refers to the chromatograms opened in that specific window. Same tab in the Calibration Report Setup refers to the calibration standard opened in the Calibration window if any. In the Instrument window it will refer to the chromatograms produced after the last run or analysis.
- Only opened chromatograms will be printed. For this reason when setting up automatic printing from *Single Analysis*, *Sequence*, *Batch* windows etc. *Open in Chromatogram Window* option must always be used as well.
- If you set up the report to be printed automatically it is always necessary to specify *Report Style* to be used.

Note: It is also possible to report multiple already measured chromatograms at once using the *Batch* dialog. See Post-run Options from Batch topic for more info.

For more info regarding reports see the **Clarity Reference Guide**.

To *Print* a Report:

1. Select *File - Print* in the *Instrument, Calibration, Chromatogram* or *Sequence* windows. In *Method Setup* click *Report Setup* icon and in the following dialog click *Print....*

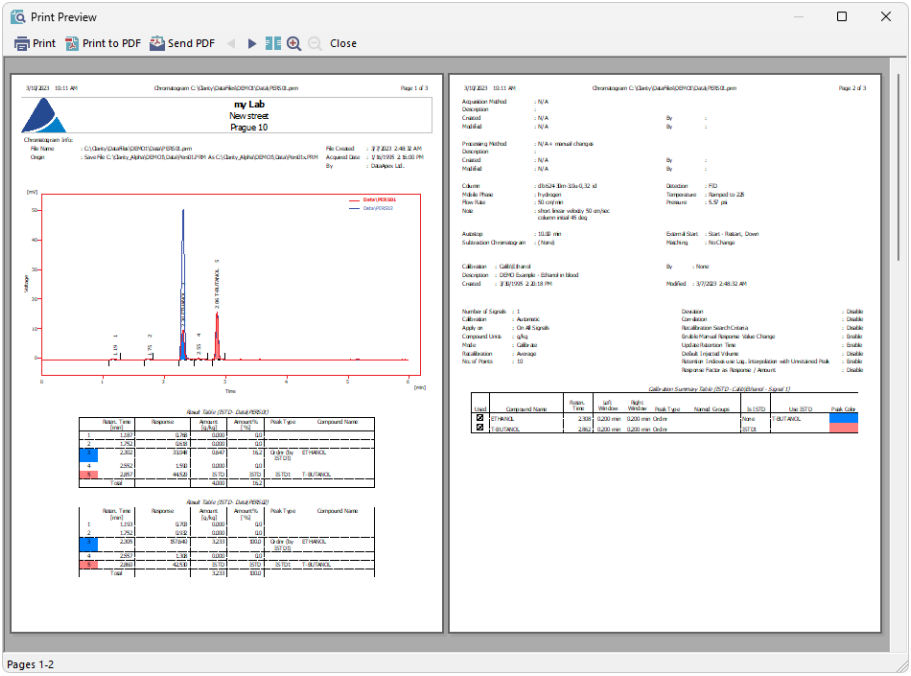
2. *Print* dialog will open for you to setup your printing options and confirm the printout.

To *Print to PDF*:

1. Select *File - Print to PDF* in the *Instrument, Calibration, Chromatogram* or *Sequence* windows. In *Method Setup* click *Report Setup* icon and in the following dialog click *Print to PDF*.
2. *Print to PDF* dialog will open for you to enter file name confirm the saving of the file.

To display *Print Preview*:

1. This feature is useful while preparing your own report style to check whether the outcome is as needed.
2. Select *File - Print Preview* in the *Instrument, Calibration, Chromatogram* or *Sequence* windows. In *Method Setup* click *Report Setup* icon and in the following dialog click *Preview...*.
3. *Print Preview* dialog will open. From there you can browse or print the report.

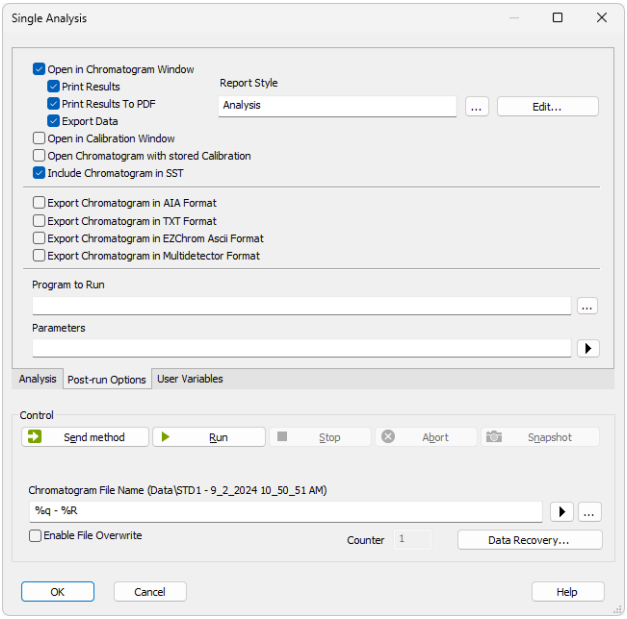


Automatic report generating after analysis is finished:

By default generated reports are placed next to the original files, to change it use *Setting - User Options* in the *Instrument* window. Navigate to *Directories* tab and specify your custom path.

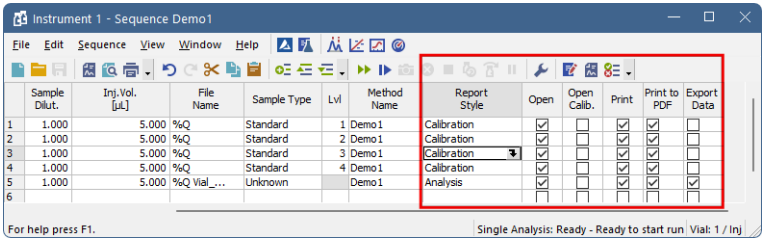
Single Analysis

1. Navigate to *Single Analysis - Post-run Options* tab.
2. Check options *Open in Chromatogram Window*, *Print Results* and/or *Print Results to PDF*.
3. Select *Report Style* by clicking ... button.
4. It is also possible automatically export data, to do so check *Export Data* option. What should be exported can be set by using *Setting - Export Data* in the *Instrument* window.



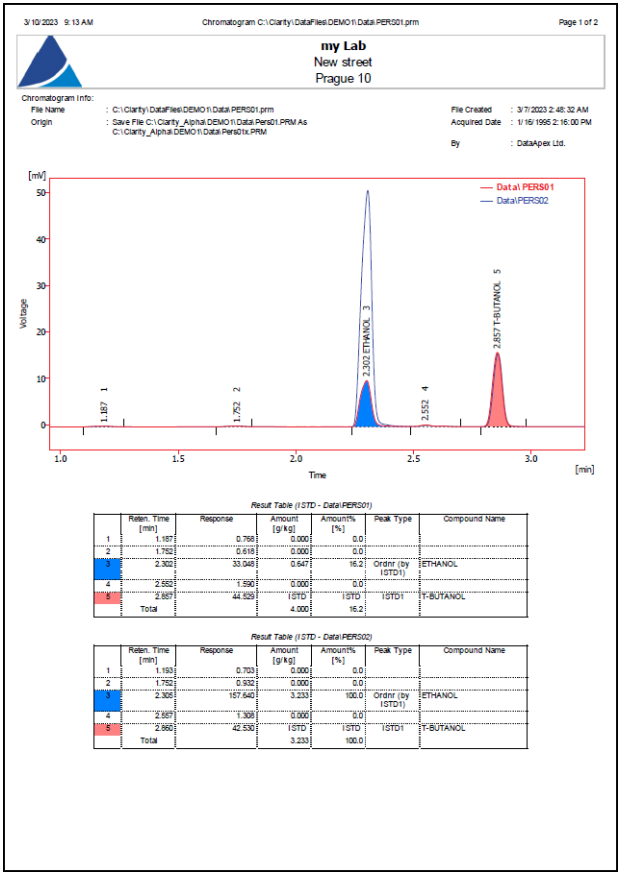
Sequence

1. Procedure is similar to the single analysis. In *Sequence* window some of the required columns are hidden by default, to display them right-click the sequence table and use *Setup Columns* in the following dialog move desired columns to the *Show Columns* list.
2. Check checkboxes in columns *Open*, *Print* and/or *Print to PDF* on rows where report should be generated.
3. Select *Report Style* for each row where report is generated. It is possible to modify specif report style by selecting its cell and clicking .
4. It is also possible automatically export data, to do so check *Export Data* option. What should be exported can be set by using *Setting - Export Data* in the *Instrument* window.



13.3 Creating a report style (example)

This is an example on how to setup a new report style to obtain the results shown in the picture. Beware that tables are printed as on screen, if e.g., calibration table is to wide to fit on one page you can adjust the column width in *Calibration* window.



3/10/2023 9:13 AM Chromatogram C:\Clarity\DataFiles\DEMO1\Data\PERS01.prm Page 1 of 2

my Lab
New street
Prague 10

Chromatogram Info:

File Name : C:\Clarity\DataFiles\DEMO1\Data\PERS01.prm
Origin : Save File C:\Clarity_Alpha\DEMO1\Data\Pers01.PRM As C:\Clarity_Alpha\DEMO1\Data\Pers01x.PRM

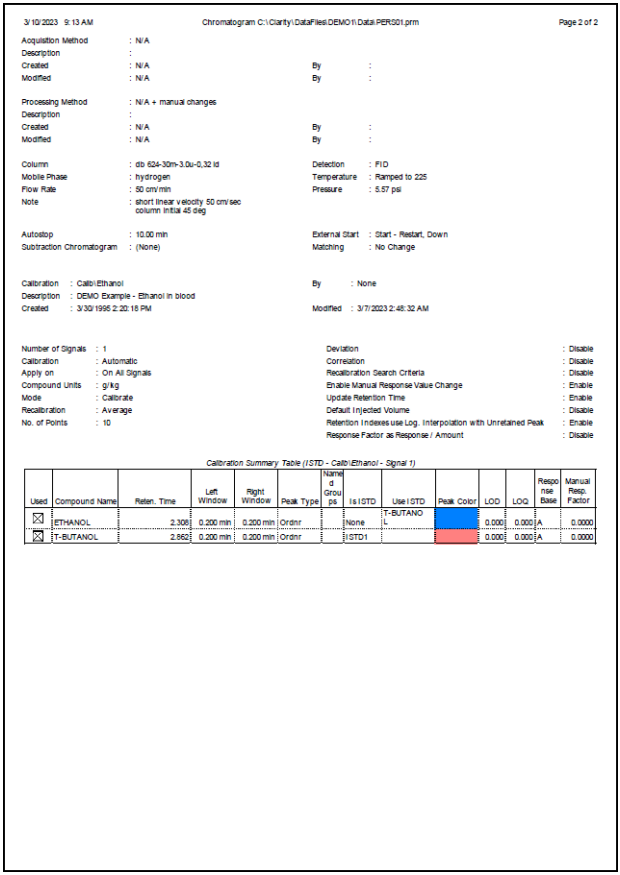
File Created : 3/7/2023 2:48:32 AM
Acquired Date : 1/16/1995 2:16:00 PM
By : DataApex Ltd.

Result Table (ISTD - Data\PERS01)

	Reten. Time [min]	Response	Amount [g/kg]	Amount% [%]	Peak Type	Compound Name
1	1.187	0.768	0.000	0.0		
2	1.752	0.618	0.000	0.0		
3	2.302	33.048	0.647	16.2	Ordnr (by ISTD1)	ETHANOL
4	2.552	1.590	0.000	0.0		
5	2.857	44.529	ISTD	ISTD	ISTD1	T-BUTANOL
	Total		4.000	16.2		

Result Table (ISTD - Data\PERS02)

	Reten. Time [min]	Response	Amount [g/kg]	Amount% [%]	Peak Type	Compound Name
1	1.193	0.703	0.000	0.0		
2	1.752	0.932	0.000	0.0		
3	2.308	157.640	3.233	100.0	Ordnr (by ISTD1)	ETHANOL
4	2.557	1.309	0.000	0.0		
5	2.868	42.530	ISTD	ISTD	ISTD1	T-BUTANOL
	Total		3.233	100.0		



3/10/2023 9:13 AM Chromatogram C:\Clarity\DataFiles\DEMO1\Data\PERS01.prm Page 2 of 2

Acquisition Method : N/A
Description :
Created : N/A By :
Modified : N/A By :

Processing Method : N/A + manual changes
Description :
Created : N/A By :
Modified : N/A By :

Column : db 624-30m-3.0u-0.32 id
Mobile Phase : hydrogen
Flow Rate : 50 cm/min
Note : short linear velocity 50 cm/sec column initial 45 deg

Detection : FID
Temperature : Ramped to 225
Pressure : 5.57 psi

Autostop : 10.00 min
Subtraction Chromatogram : (None)

External Start : Start - Restart, Down
Matching : No Change

Calibration : Calib\Ethanol
Description : DEMO Example - Ethanol in blood
Created : 3/30/1996 2:20:16 PM

By : None
Modified : 3/7/2023 2:48:32 AM

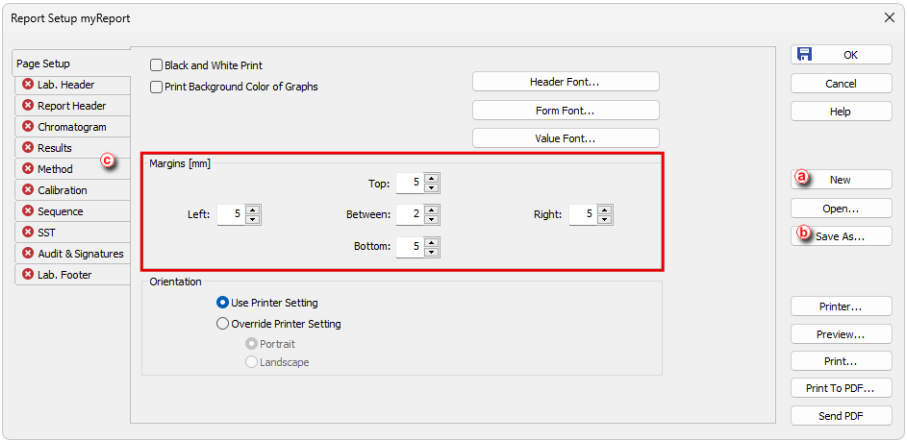
Number of Signals : 1
Calibration : Automatic
Apply on : On All Signals
Compound Units : g/kg
Mode : Calibrate
Recalibration : Average
No. of Points : 10

Deviation : Disable
Correlation : Disable
Recalibration Search Criteria : Disable
Enable Manual Response Value Change : Enable
Update Retention Time : Enable
Default Injected Volume : Disable
Retention Indexes use Log. Interpolation with Unretained Peak : Enable
Response Factor as Response / Amount : Disable

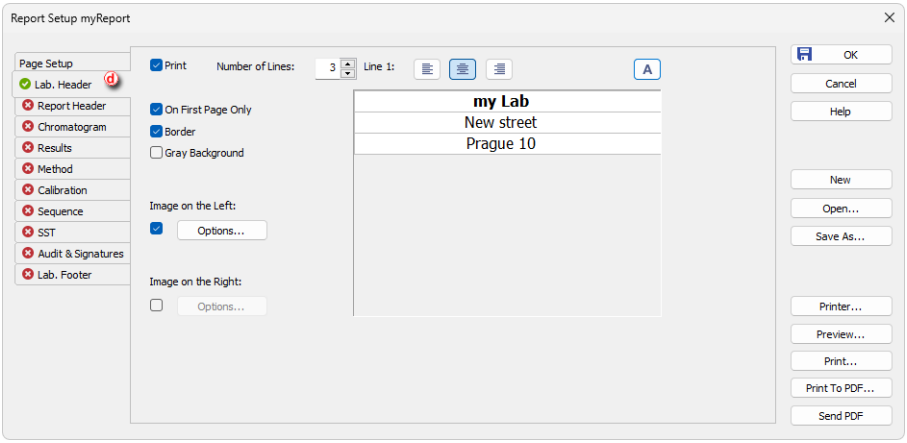
Calibration Summary Table (ISTD - Calib\Ethanol - Signal 1)

Used	Compound Name	Reten. Time	Left Window	Right Window	Peak Type	Named Groups	Is ISTD	Use ISTD	Peak Color	LOD	LOQ	Response Base	Manual Resp. Factor
☒	ETHANOL	2.306	0.200 min	0.200 min	Ordnr		None	T-BUTANOL		0.000	0.000	A	0.0000
☒	T-BUTANOL	2.662	0.200 min	0.200 min	Ordnr		ISTD1			0.000	0.000	A	0.0000

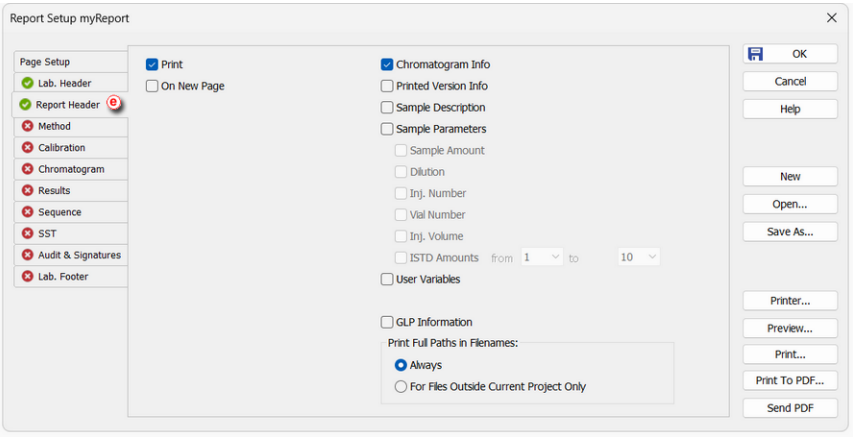
1. Open the chromatograms PERS01 and PERS02 in overlay (located in C:\CLARITY\DATAFILES\DEMO1\DATA).
2. Select the graph area you want to print by clicking and dragging the cursor in the chromatogram graph.
3. Create a new report style.
   - Select the *File - Report Setup*.
   - Click on the *New* button ⓐ to create a new report style.
   - Click on the *Save As...* button ⓑ and save the style under the name (*myReport* in this example).
4. Click and drag the tabs ⓒ to set them in desired order. This will be the order the sections will have in the report.
5. Set the *Margins* as needed.



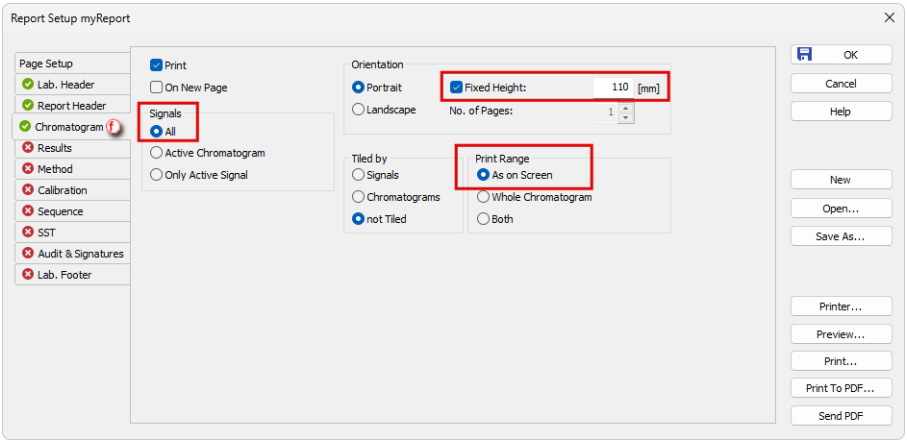
6. Set the *Lab Header*.
    - Click the *Lab Header* tab ⓓ .
    - Check the checkboxes *Print*, *On First Page Only* and *Border*.
    - Check the *Image on the Left* checkbox and click on the *Options...* button to select the logo.
    - Click in each line in the text box and write the you want to have in the header.
    - Click in the first line of text and then on the *Font* icon (icon with "*A*") and select *Bold* as a *Font Style*.



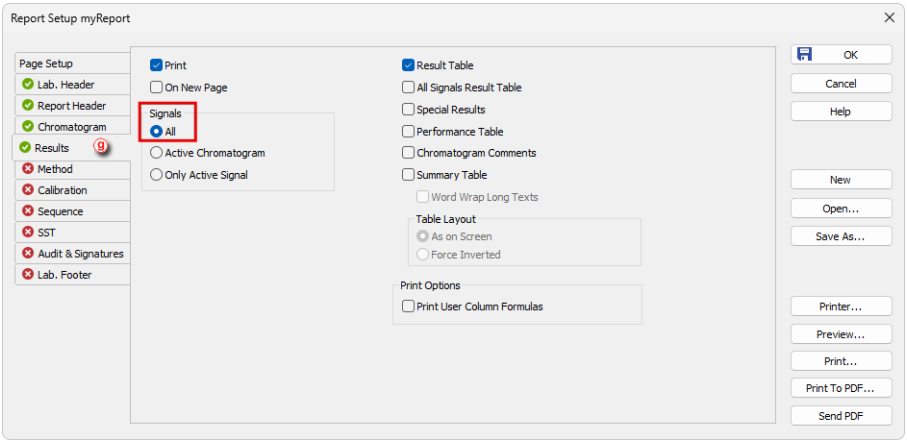
7. Set the *Report Header*.
    - Click the *Report Header* tab ⓔ .
    - Check the options *Print* and *Chromatogram Info*.



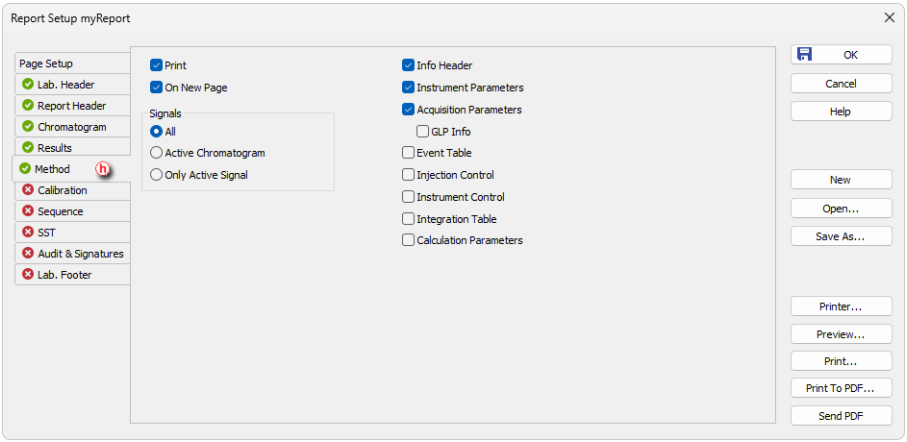
8. Set the *Chromatogram section*. Only the format of printed graphs is set here, result tables are printed based on *Results* tab, see next step.
    - Click the *Chromatogram* tab ⓕ .
    - Check the options *Print* and *Fixed Height* and set the height to 110 mm.
    - Select the options *Signals - All* and *Print range - As On Screen*.



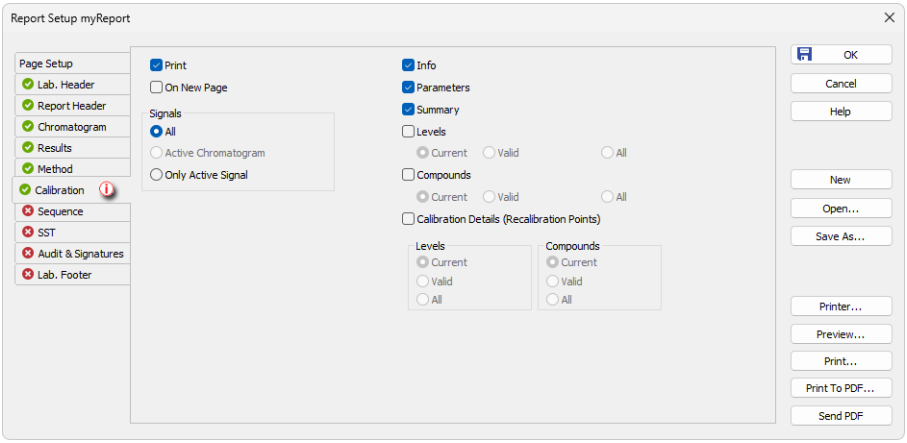
9. Set the *Results* section.
    - Click the *Results* tab ⓖ .
    - Check the options *Print* and *Result Table*.
    - Select the option *Signals - All*.



10. Set the *Method* section.
    - Click the *Results* tab. ⓗ
    - Check the options *Print*, *On New Page*, *Info Header*, *Instrument Parameters* and *Acquisition Parameters*.
    - Select the option *Signals - All*



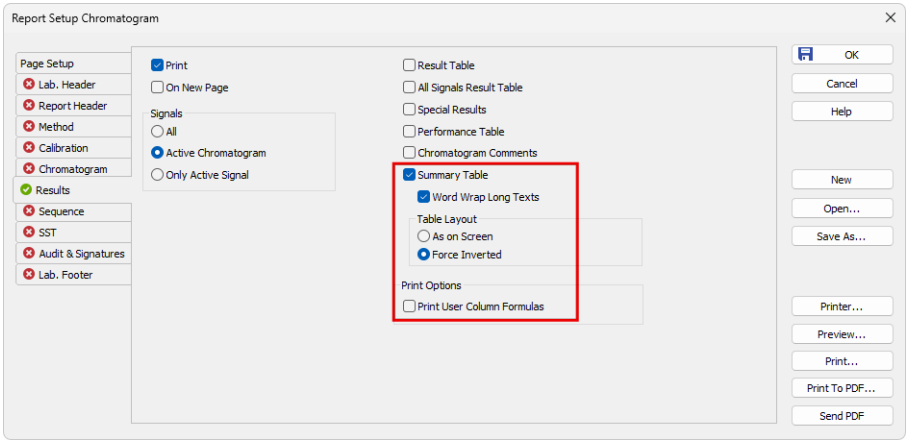
11. Set the *Calibration* section.
    - Click the *Calibration* tab ⓘ .
    - Check the options *Print*, *Info*, *Parameters* and *Summary*.



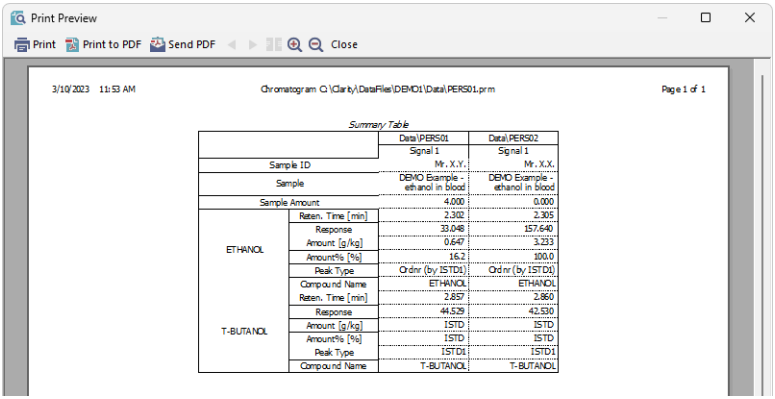
12. You can preview your report by clicking *Preview...*. For more info see ***Printing or previewing a report***.
13. Click the *OK* to save the report style.

13.4 Printing the summary table

1. Setup *Summary* table in *Chromatogram* window. For information on how to create Summary Table, see the chapter **"Comparing the results from several chromatograms"** on pg. **173**.
2. Right-click in the *Summary Table*, if you want to change the visualization of the table, add a custom column, etc.
3. Open the *Report Setup* dialog and check the *Summary Table* checkbox in the *Results* tab.
4. It is also recommended selecting *Word Wrap Long Texts* and *Force Inverted* (table will be printed with inverted layout ignoring the on-screen layout which is more suitable for reports) options. *Print User Column Formulas* can be used when custom columns are included in the table.



5. The results for all opened chromatograms will be printed.



14 File Management

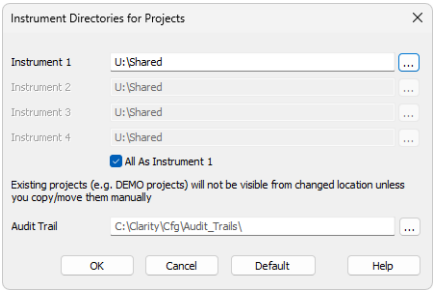
How to set project directories, create new projects, preset file names of measured chromatograms based on variables, store files into subfolders etc.

14.1 Setting up project directories

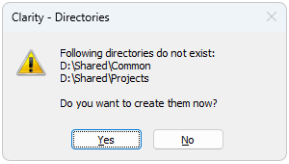
It is possible to set different directories for projects accessible from each instrument and to set the Audit Trail directory. This is useful while working with a shared disk if it is necessary to access measured data from another PC using **Clarity Offline**.

To setup a custom project directories do following:

1. Open Main **Clarity** window.
2. Open the *Instrument Directories for Projects* dialog using the *System - Directories...* command or the icon.



3. Set the desired directory e.g., *U:\Shared*.
4. If needed, change the *Audit Trail* directory as well.
5. When saving the changes, the following dialog may appear. Confirming it will create the necessary subfolder structure in your target location. COMMON is filled by default files that are necessary for functioning.



Given that a new COMMON directory has to be created in the custom directory, the report styles and templates for a new method, calibration, and sequence become instrument-specific.

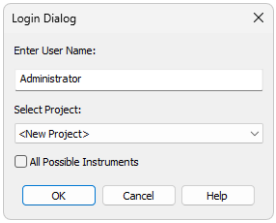
Caution: Be aware that when updating Clarity the COMMON files outside of the installation directory must be updated manually.

14.2 Creating a new project

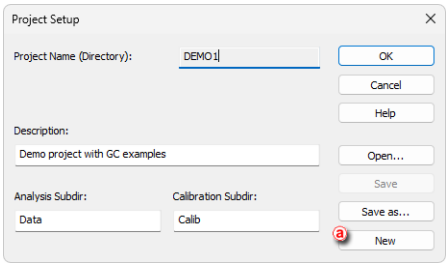
Creating a new project ensures that the measured data will be later easily found. The project itself is a directory in **Clarity's** DATAFILES subfolder or selected directory where all relevant files are saved (methods, calibrations, sequences, chromatograms).

1. To create new project navigate to the *Project Setup* dialog by selecting *Instrument - Project...* in the *Instrument* window.

Note: You can also open a project through the *Login Dialog* opened from the Main Clarity window by selecting the *New Project* option and clicking OK.

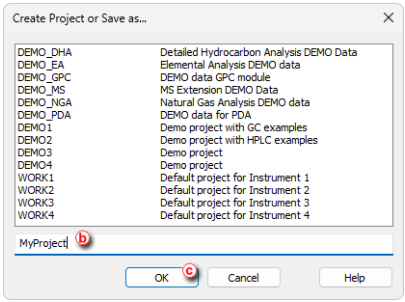


2. In the *Project Setup* dialog click the *New* button ⓐ to create a new project.



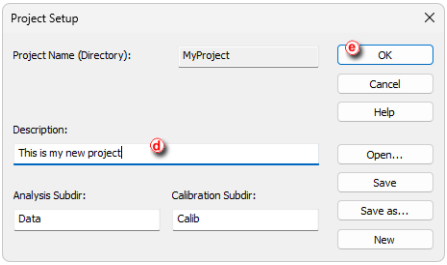
3. Set the name of the new project ⓑ and click *OK* ⓒ .

Note: Entered project name must not contain invalid characters, i. e. \ /:*?"< >|.



4. Fill in the project description in the *Description* field ⓓ and click *OK* ⓔ .

Note: The change of the project will require you to restart the Instrument. If there are any unsaved files opened, you will be prompted to save them. The newly created project does not include any files (for example method, calibration etc.).



14.3 Creating customized file names automatically

You can create customized file names automatically by appending variables to them.

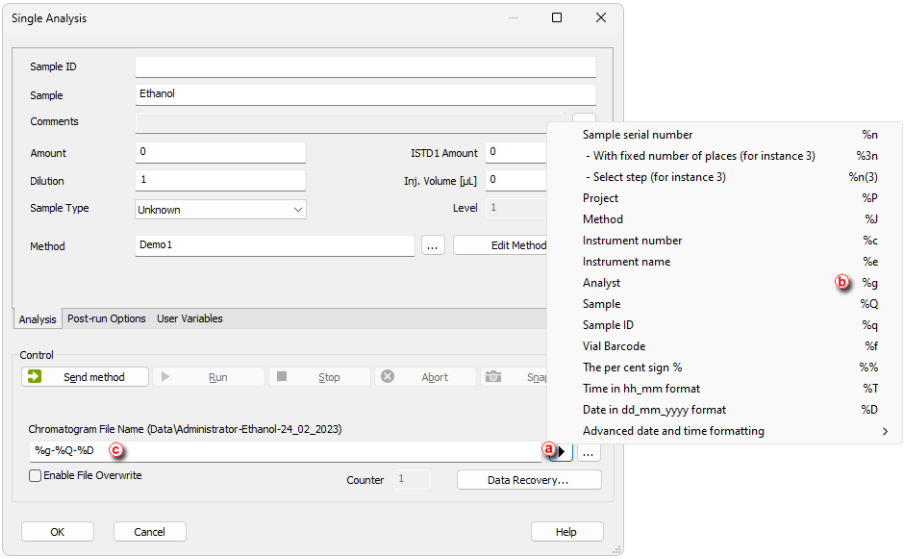
File names can be created in the *Single Analysis* window, in the *Sequence* window and on the *Method Setup - Calculation* tab.

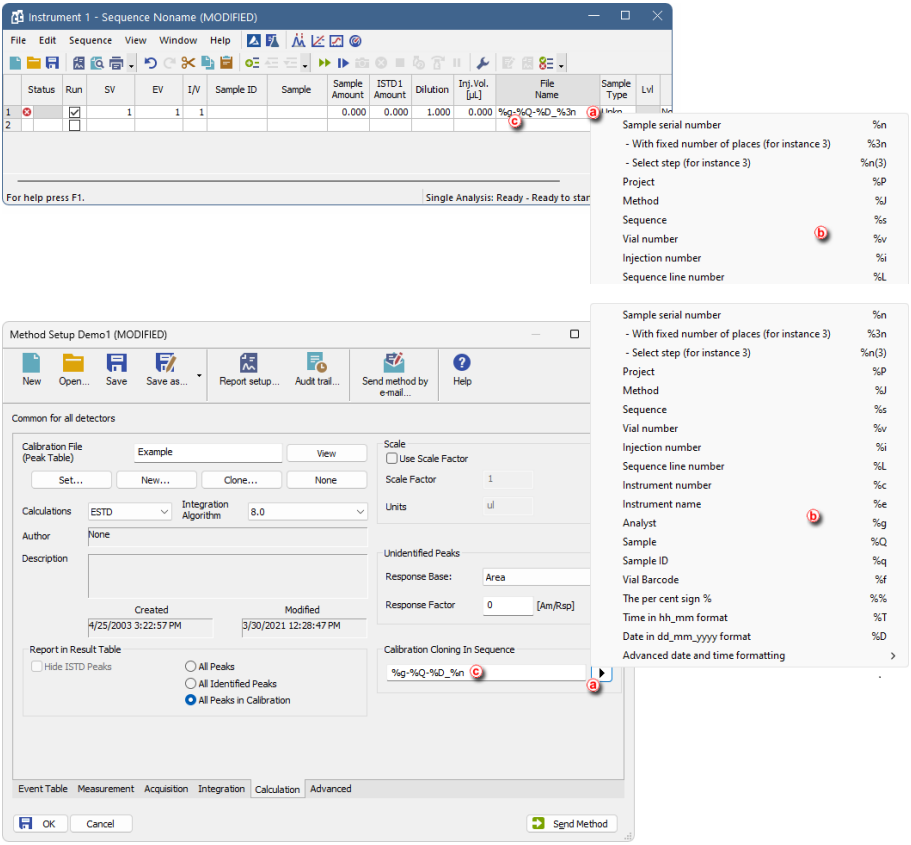
1. Click on the respective icons , , in the *Instrument* window to open the *Single Analysis*, the *Sequence* or the *Method Setup - Calculation* window.
2. Click on to open the variable list. ⓐ
3. Select the variable you want to include in the file name. ⓑ
4. Repeat the previous two steps to add more variables.

5. Insert any allowed characters between the variables to create your file name. ©

More Info:

- Variables are preceded by the "%" character and they are substituted by their value upon file creation. For example "*%g-%Q-%D*" will create a file name with the name of the *Analyst*, the *Sample* and the *date*: "*Administrator-Ethanol-24_02_2023.prm*".
- To prevent an *Unresolved File Name* error you can append the *Sample Serial Number* "%n" or the date and time "%R".


Single Analysis
Sample ID
Sample
Ethanol
Comments
Amount
0
ISTD1 Amount
0
Dilution
1
Inj. Volume [µL]
0
Sample Type
Unknown
Level
1
Method
Demo1
Edit Method
Analysis
Post-run Options
User Variables
Control
Send method
Run
Stop
Abort
Chromatogram File Name (Data\Administrator-Ethanol-24_02_2023)
%g-%Q-%D
Enable File Overwrite
Counter
1
Data Recovery...
OK
Cancel
Help
Sample serial number %n
- With fixed number of places (for instance 3) %3n
- Select step (for instance 3) %n(3)
Project %P
Method %J
Instrument number %c
Instrument name %e
Analyst %g
Sample %Q
Sample ID %q
Vial Barcode %f
The per cent sign % %%
Time in hh_mm format %T
Date in dd_mm_yyyy format %D
Advanced date and time formatting
a
b
c



14.4 Storing chromatograms into subfolders

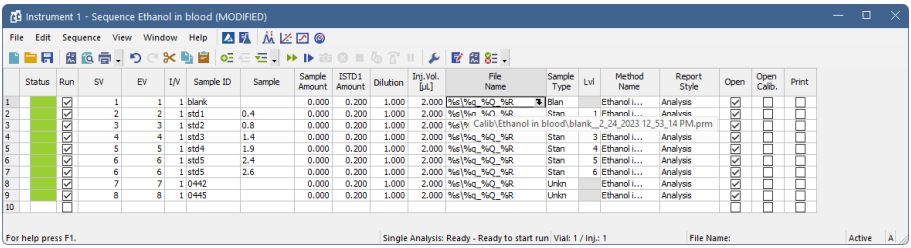
It is possible to include the name of a subfolder in the *File name* to store chromatograms into project's subfolder. If the subfolder doesn't exist, it will be created when the chromatogram is stored. The directory can be set using the **"\"** character. Any string of the variables or characters in front of the **"\"** character is considered as the subfolder name. Any string of variables or characters after the **"\"** character is used as the file name.

Subfolders created this way are present in DATA and CALIB subfolders of used project.

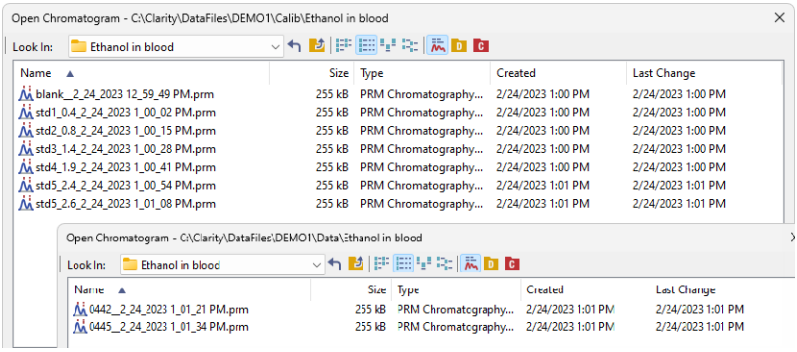
Here we provide an example on how to store chromatograms from one sequence into subfolder named after it.

1. Login to *Instrument* with DEMO1 project.
2. Open the *Sequence* window.
3. Open ETHANOL IN BLOOD.SEQ.

4. Set the File Name of the first row to **%s\%q_%Q_%R**. (To see detailed description on how to create the name using variables see chapter "Creating customized file names automatically" on page 193.)
5. Right click on the *File Name* column and select *Fill down* to apply the name to all rows.



6. The Chromatogram file with a name of SAMPLEID_SAMPLE_DATE-AND-TIME will be stored in *Demo1\Data\Ethanol in blood* folder for unknown samples and in *Demo1\Calib\Ethanol in blood* folder for standards and blank.



- To create subfolder for each month use the %m or %B variables and for each day use the %a or %A variables.
- Same procedure can be also used in *Single Analysis* window.

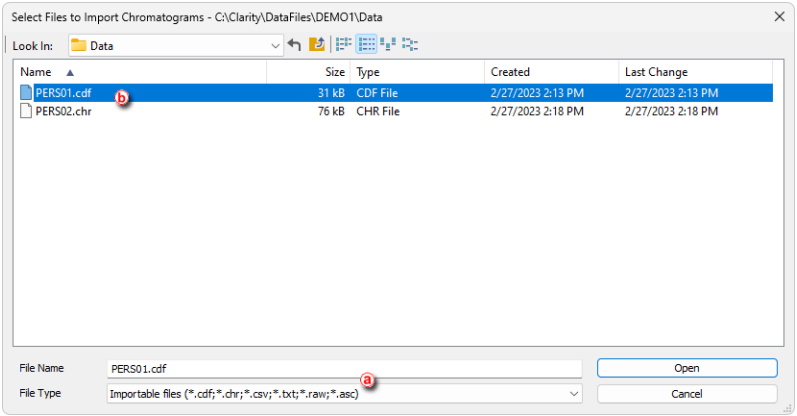
15 Import and Export Data

Clarity allows to import or export chromatograms from/to various formats. Following chapters describe you how to, for example, set exporting chromatograms to a LIMS.

15.1 Importing a chromatogram into Clarity

It is possible to import chromatograms from other chromatography software. Supported formats are : AIA (*.CDF suffix), EZChrom ASCII (*.ASC suffix), Text format (*.TXT), Comma Separated Values format (*.CSV) or Multi-detector format (*.CHR). The particular procedure depends on type of file you want to import.

1. From the *Chromatogram* window open the *Open Files To Import* dialog by selecting *File - Import Chromatogram…*.
2. You can select the *File Type* which you want to import ⓐ . By default you can see all supported formats.
3. Select the file(s) you want to import ⓑ and click on the *Open* button.



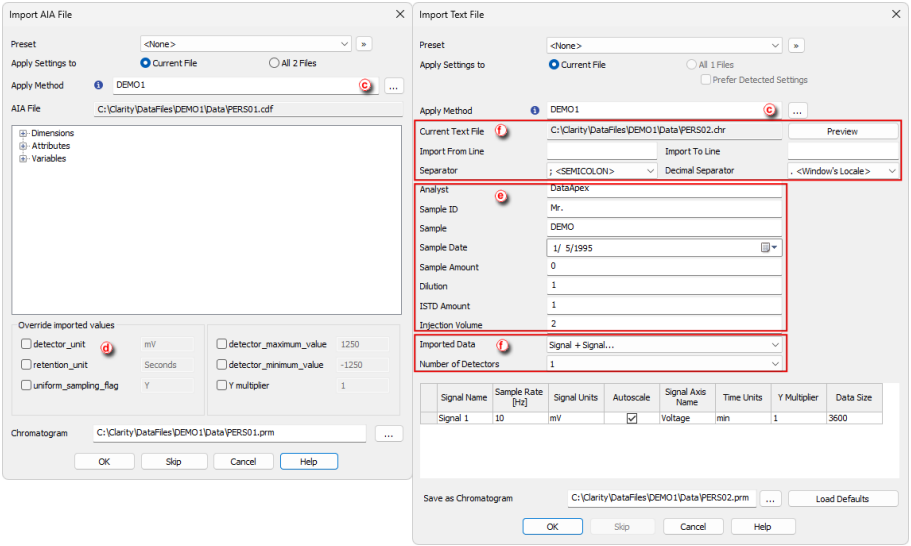
4. Set the parameters as needed in the subsequent dialogs depending on the file format.
5. For all file formats you can select imported file name and which method to apply ⓒ . This will apply integration, calibration etc.

- Import AIA File - when importing AIA file (*.CDF suffix).
  - You have option to inspect data from the source file and override some of them ⓓ e.g, *Detector Unit*.
- Import Text File - when importing Text, Multidetector or EZChrom ASCII file (*.TXT, *.CHR, *.ASC and *.CSV suffixes).
  - You can set information regarding given sample ⓔ like *Dilution* or *Injection Volume* etc. You can also set information regarding source file

format ⓕ .

Note: File format related settings is typically detected automatically and there is no need to change it.

- *Save As* - when importing *.RAW file, as there is no need to set other parameters.



15.2 Exporting a chromatogram from Clarity to a different chromatography data station

It is possible to export chromatograms to other formats used by chromatography data stations. The supported formats are : *AIA* (*.CDF suffix), *EZChrom ASCII* (*.ASC suffix), *Text format* (*.TXT), or *Multi-detector format* (*.CHR).

1. Open the *Chromatogram* window by selecting *Window - Chromatogram* on the *Instrument* window or click on .
2. Open the chromatogram you want to export, then open the *Export Chromatogram* dialog by selecting *File - Export - Export Chromatogram….*
3. Select the export format ⓐ . Notes:

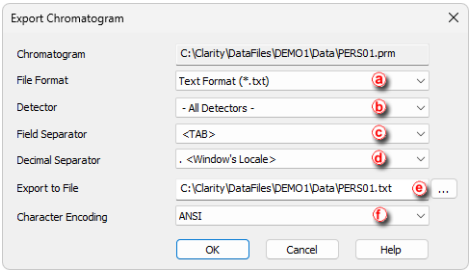
   Note: For PDA export of 3D data only the EZChrom ASCII format is supported.

4. Select the signals to be exported ⓑ .

   Note: You can choose individual signals, *All Detectors*, *3D Data* or *All Detectors + 3D Data* (3D Data variants in EZChrom ASCII only).

5. Select the field separator character ⓒ .

6. Select the decimal separator character ⓓ .
7. Open the *Export Chromatogram As* dialog clicking on ... . Enter the name and location of the file into which you wish to export the chromatogram ⓔ or fill in the file name.
8. Select the character encoding for the exported file (*ANSI* or *Unicode (UTF-8)*) ⓕ .
9. Click *OK* to finish the export.



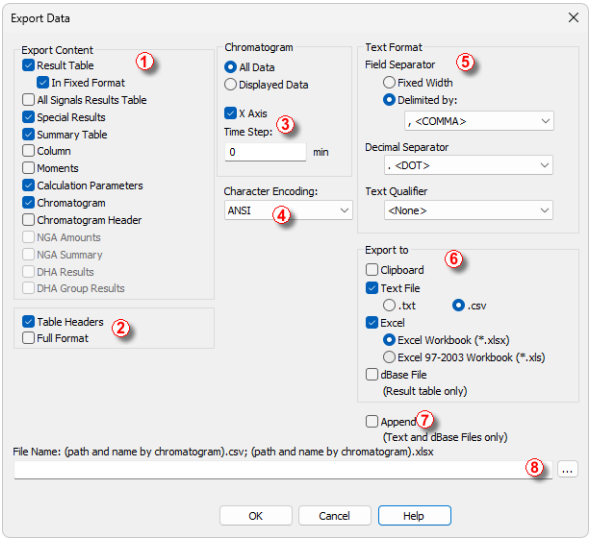
15.3 Exporting data from Clarity

It is possible to export selected parts of the results into external files. All of this can be achieved automatically from *Sequence* or *Single Analysis* window by selecting *Export Data* in *Post-run Options* or manually from the *Chromatogram* window.

1. Open *Export Data* dialog from *Instrument* window by using *Setting - Export Data...*
2. Select which data you want to include in the exported files in the *Export Content* group ① . Detailed description of these fields can be found in the Reference Guide.
3. Select whether you want the tables exported with headers and/or in the full format ② .
4. Select whether the exported chromatogram data will contain time column or not. If you intend to perform bunching for the exported data specify the time period for the bunching ③ .

   Note: The mean value for selected *Time step* period is calculated as a sum of the highest Y_{Max} and lowest Y_{Min} signal curve value found within each *Time Step* period divided by two - $(Y_{Max}+Y_{Min})/2$.

5. Select the character encoding to be used (*ANSI* or *Unicode (UTF-8)*) ④ .
6. Select the appropriate text formatting for the export ⑤ .
7. Select the format or formats to which the data will be exported. You can choose any number of export types at the same time ⑥ .
8. Select whether the exported data should be appended into an existing file ⑦ (in this case file name ⑧ must be filled in) or exported as a new file (leave the file name empty as shown bellow).



- This setting will be used for automated data export from *Sequence* or *Single Analysis*.
- To manually export data you can invoke the same dialog from *Chromatogram* window by using *File - Export - Export Data...* command or icon. In this case dialog also includes *Export* button which can be used the export data from currently opened chromatogram.

15.4 Exporting data for LIMS

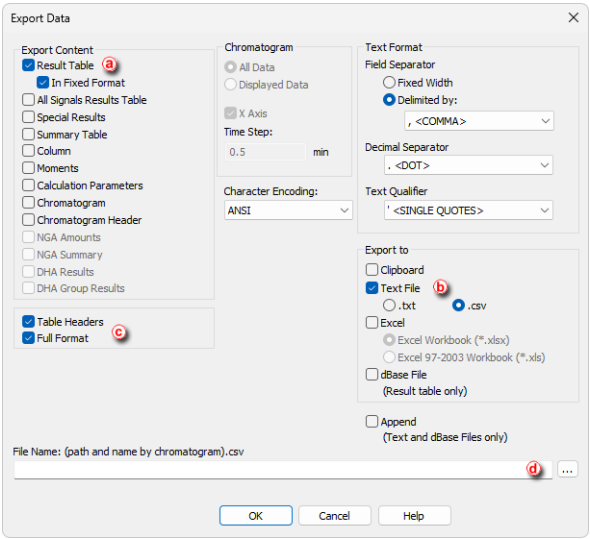
Following chapter describes how to export data from Clarity to be used for LIMS. Each LIMS requires a different approach in importing external data, therefore it may be necessary to adjust your LIMS to be able to correctly process imported data from Clarity.

Export settings

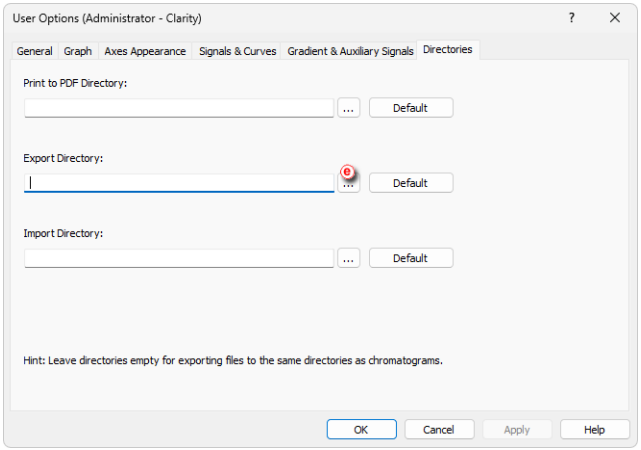
1. Open Clarity *Instrument* window and select - *Setting - Export Data...*.
2. In the *Export Data* dialog set the required *Export Content* ⓐ .

   Note: While exporting *Result Table* it is recommended to check *In Fixed Format*. Otherwise the content will change according to changes on screen. Beware that *In Fixed Format* is only applied to the *In Result Table*.
3. Select desired file formatting in *Text Format* section.
4. Select *Export to - Text File* ⓑ and choose preferred suffix.
5. Select *Full Format* option ⓒ . This will precede each result table row with a file name, date and time, thus allowing easy sorting after import.

6. Set *File Name* ⓓ and check *Append* option, in this way all results will be exported to a single file which can then be simply imported directly to your LIMS. Alternatively, leave the field empty in which case each export will be performed to a separate file. Exported files will have automatically generated file name from the chromatogram name.



- By default, files are exported to the same directory as the original chromatogram.
- To export to a single directory, specify it in the *User Options - Directories* tab ⓔ, accessible from the *Instrument* window by *Setting - User Options...* command.



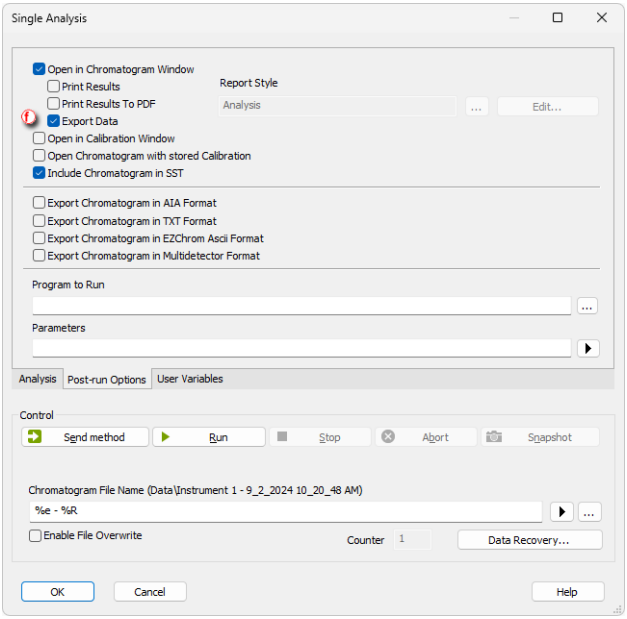
Locations to Export from

Three most common locations in exporting data to LIMS are:

Single Analysis

- In the *Post-run Options* tab of the *Single Analysis* dialog, select *Export Data* ⓕ .

Note: Export of data will be performed automatically after a single analysis is finished.



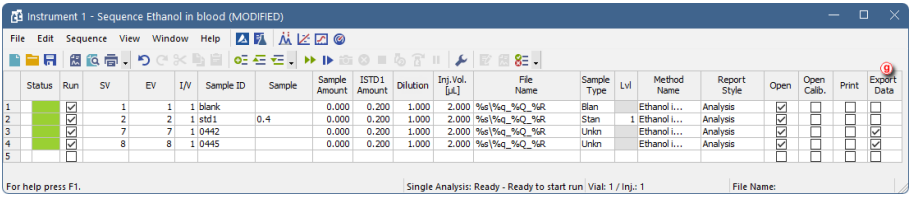
Sequence

- In the *Sequence* window, select checkbox in the *Export Data* ⓖ column for row(s) to be exported.

  Note: Export of data will be performed automatically after the row has been measured.

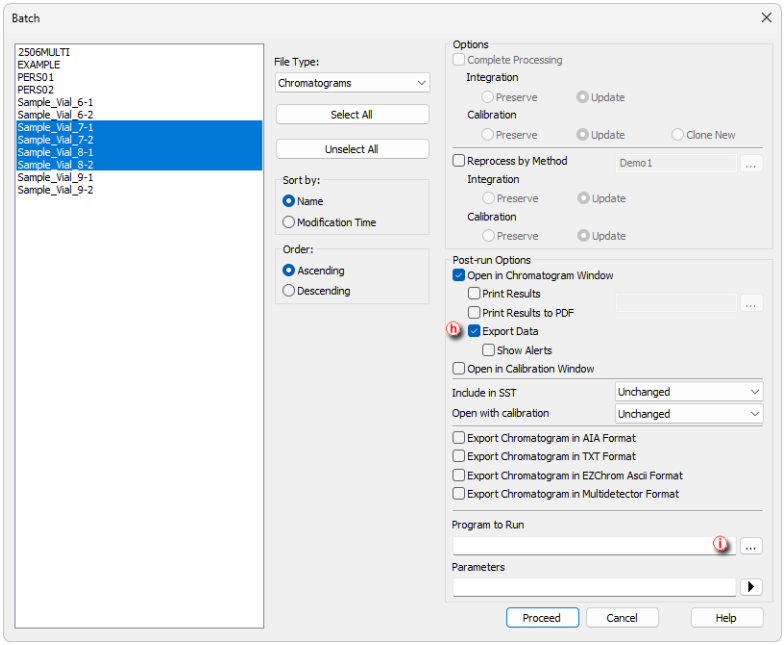
  More Info:

  - By default, *Export Data* column is hidden. Right mouse click in the sequence table and choose *Setup Columns...* to show it.
  - In the *Setup Columns* dialog, choose *Export Data* from the left list and click on the *Show* button - it will be added to the show list. Once you click on the *OK* button, you will return to the *Sequence* window and new *Export Data* column will be present.



Batch

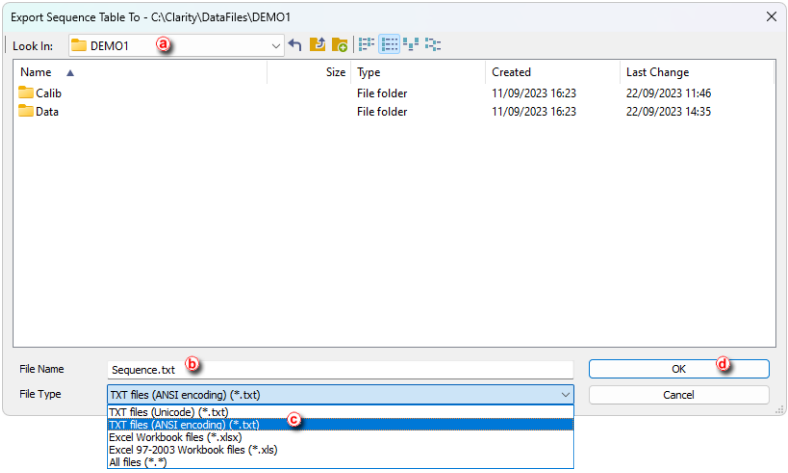
- Export multiple chromatograms at once using the *Batch* dialog, accessible from the *Instrument* window by *Analysis - Batch...* command.
- Select chromatograms to be exported and check the option to *Export Data* ⓗ .
- Clarity is able to start external program with a parameter ⓘ . Specify a program to run using the … and specify a command line parameter - typically the file name of the exported text file *%e*. Once ready to export the data, click the *Proceed* button.



15.5 Exporting sequence

It is possible to export sequence to other more common formats. Supported formats are *Excel Table* (*.XLSX and *.XLS suffixes) or *Text format* (*.TXT).

1. Open the sequence you want to export, then use the *File - Export…* command to open the *Export Sequence Table To* dialog.
2. Select the appropriate folder for saving the exported sequence ⓐ .
3. Fill in the name under which the exported sequence will be saved ⓑ .
4. Choose the format in which you want to export ⓒ . For Text format, the *ANSI* or *Unicode* encoding are available.
5. Press the *OK* button to perform the export ⓓ .

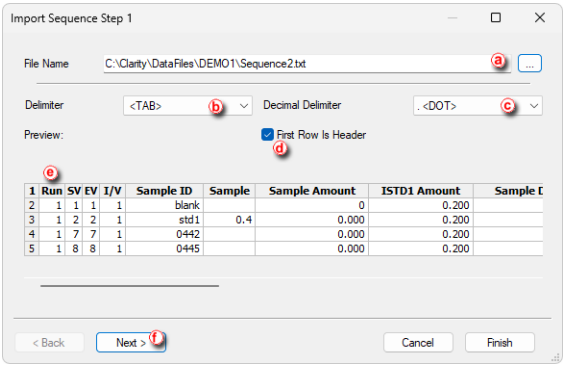


15.6 Importing sequence

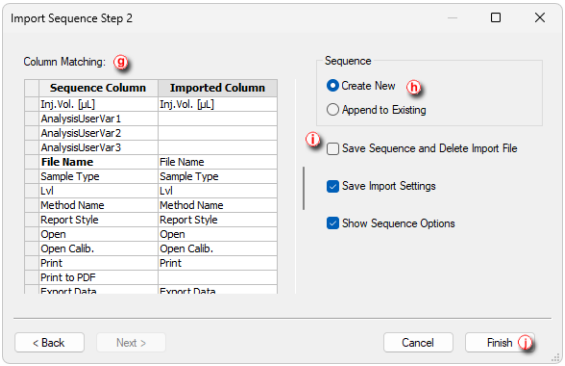
It is possible to import sequence that has been stored in a text file. Values have to be in delimited format and separated by an arbitrary delimiter.

Import of the sequence is one of the functions that enables an interconnection between Clarity and **LIMS** systems.

1. Open an Import dialog (*File - Import…*) from the *Sequence* window.
2. Choose the file which you want to import ⓐ . Supported formats are : .TXT, .CSV and .PRN
3. Select the character used as field delimiter ⓑ . Possible options are <*TAB*>, <*SPACE*>, <*COMMA*> or <*SEMICOLON*>.
4. Select the character used as decimal delimiter ⓒ . Options for the decimal delimiter are <*Window's Locale*> (the station will use the setting specified in the local settings of MS Windows), <*COMMA*>, <*DOT*> or <*SEMICOLON*>.
5. If the text file to be imported contains column descriptions in the first row, use *First Row Is Header* ⓓ checkbox. This row is used for mapping in the *Import Sequence Step 2* dialog.
6. Preview of the first five rows of the imported sequence table is displayed in the bottom part of the dialog ⓔ .
7. Click *Next* to continue ⓕ .



8. Set the mapping so that the columns used in Clarity (*Sequence Column*) will correspond to the columns from the imported file (*Imported Column*) ⓖ . Columns that are highlighted in bold letters are required. When the imported table contains column headers (the *First Row is Header* checkbox from the *Import Sequence Step 1* dialog has been checked), **Clarity** will attempt to automatically map the columns according to their names. Manual mapping will override the default name mapping. **Clarity** will store these names for future imports .
9. Select whether you want to save imported sequence as a new file or just append it to currently opened one ⓗ .
10. Three checkboxes allows you to do following ⓘ :
    - Original file will be erased after successful import.
    - Settings of this dialog will be saved for future imports.
    - Sequence Option will be shown immediately after finishing import.
11. Press the *Finish* button to accomplish import and close the dialog ⓙ .



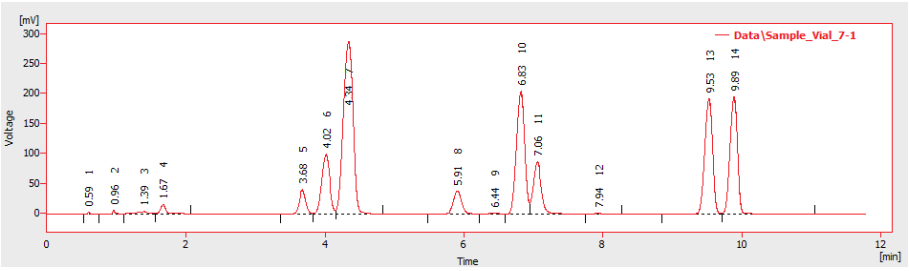
15.7 Exporting a chromatogram as a picture

You can export a chromatogram as a picture to the clipboard or as a file to a folder of your choice. The picture will include the labels and lines included in the chromatogram.

1. Open the *Chromatogram* window by selecting *Window - Chromatogram* from the *Instrument* window or click on .
2. Open the chromatogram you want to export.
3. Select *File - Export - Export as picture to clipboard* and paste the picture to MS Word, MS Powerpoint, Open Office Writer or any other suitable application of your choice.

   or

4. Select *File - Export - Export as picture to file...* and then select the folder where you would like to save the file in *Enhanced Metafile Format*.



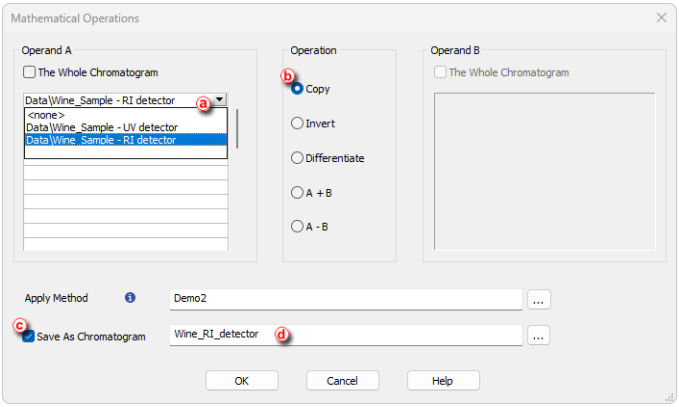
16 Mathematical Operations

This functionality was implemented into Clarity to give users a tool to manipulate already measured data without modifying original raw data. Mathematical operations present a very convenient approach to perform various actions such as extraction of a selected signal(s) from multiple signal chromatogram or subtraction of various chromatograms from each other. You can display three examples of applications of *Mathematical Operation* in following chapters. Many other applications may be developed by Clarity users on their own.

16.1 Extract chromatogram's signal using Mathematical Operations

You can save a particular signal from a chromatogram that contains several of them. This results in a stand-alone chromatogram file containing only the individual signal of choice, not all of the signals from the original chromatogram which might be confusing when working with a larger number of signals.

1. Open your a multi-signal chromatogram that you want to work with.
2. In *Chromatogram* window select *Chromatogram - Overlay - Mathematics* to open *Mathematical Operations* dialog.
3. From the drop-down menu ⓐ in the *Operand A* section select the desired signal of chromatogram you want to save separately. Select the *Copy* operation ⓑ , check *Save As Chromatogram* ⓒ , fill a name of the new chromatogram ⓓ and click *OK* to save the signal as standalone chromatogram.

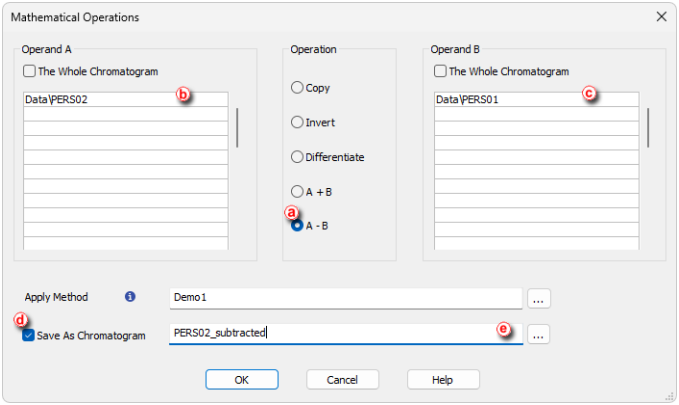


16.2 Subtraction of various chromatograms using Mathematical Operations

If you would like to use one of your chromatograms as a baseline for another chromatogram(s) there is a way to subtract the desired chromatogram from any

other chromatogram. It is possible to set *Subtraction Chromatogram* directly in *Chromatogram* window on *Measurement Conditions*, however, if you want to have both original and subtracted chromatograms as individual files you can use *Mathematical Operations*.

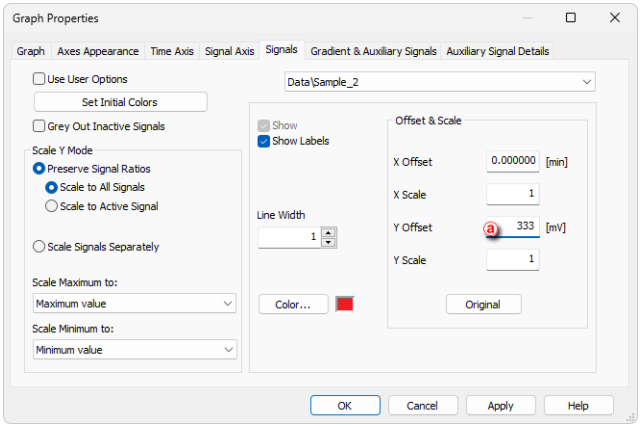
1. Open your chromatograms that you want to work with in *Overlay*.
2. In *Chromatogram* window select *Chromatogram - Overlay - Mathematics* to open *Mathematical Operations* dialog.
3. Select operation *A - B* ⓐ . From the drop-down menu in the *Operand A* section, select the chromatogram you want to subtract from ⓑ .
4. From the drop-down menu in the *Operand B* section, select the chromatogram you want to subtract ⓒ .
5. Check span *Save As Chromatogram* ⓓ , fill a name ⓔ and click *OK* to save the new subtracted chromatogram.



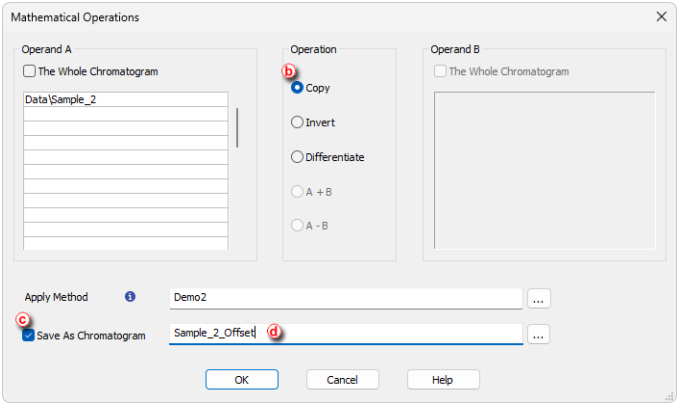
16.3 Copying of chromatogram using Mathematical Operations

Following chapter describes how to copy a modified chromatogram into a new one without changing the original chromatogram. For example we set up new Offset of Y-axis and this modification is about to saved in new chromatogram and want to keeping the original chromatogram unchanged.

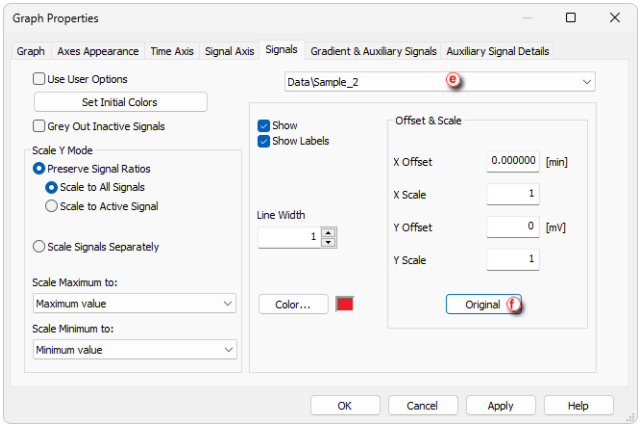
1. Open your chromatogram that you want to work with.
2. In *Chromatogram* window click *Display - Properties* to open *Graph Properties* and go to *Signals* tab.
3. Into Field *Y Offset* ⓐ write down value of desired offset in mV, in this example we choose 333 mV, and click *OK* button.



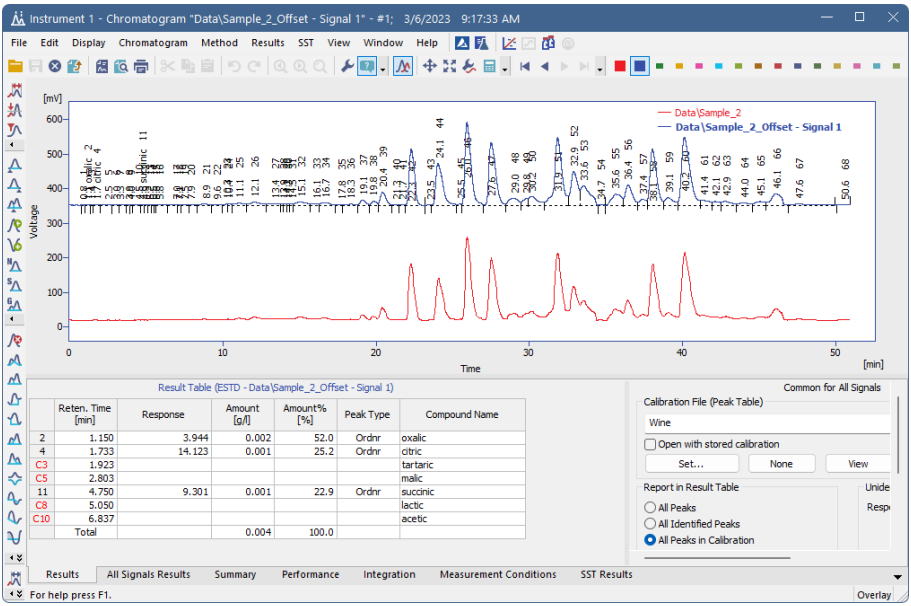
4. Select *Chromatogram - Overlay - Mathematics...* and the *Mathematical Operations* window will open.
5. Select *Copy* option ⓑ. Check *Save as Chromatogram* ⓒ, name the new chromatogram ⓓ and click the *OK* button.



6. Both chromatograms will be displayed in overlay mode.
7. Restore the original chromatogram by navigating to *Graph Properties - Signals* as in step 2.
8. Select the original chromatogram ⓔ, click *Original* button ⓕ and close the dialog by clicking *OK*.



9. Both chromatograms will be displayed in overlay mode as shown in the next image.



17 Archive and Restore

Clarity allows you to archive your PROJECTS (methods, sequences, measured chromatograms) and also the COMMON folder in which the print styles are stored.

17.1 Archiving a project (Creating an Archive)

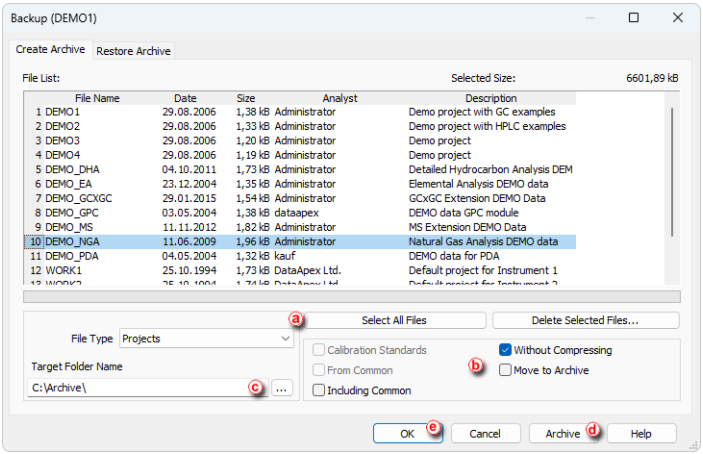
It is strongly recommended to archive the whole project folder after being shelved, but it is also possible to archive specific files only. An archive can be made by simply copying the files or by compressing them into one file (*.DGZ format).

1. Open the *Backup* dialog by selecting *Instrument- Archive...* on the *Instrument* window.
2. Select *Projects* in the *File Type* ⓐ option to archive a complete project directory.
3. Select the project or projects you wish to back up from the list. The *Select All Files* button ⓐ will select all projects.
4. Choose from the following options ⓑ :
    - Uncheck the *Without Compressing* option to archive all files into one compressed file.
    - Check the *Move to Archive* option to have the original files erased after backing them up.
    - Check the *Including Common* option to also back up the COMMON subdirectory.
5. Choose the output directory and name for the archive ⓒ . Compressed files will have the .DGZ extension.

    Caution: If you archive data in compressed format with a previously used name, you can possibly override the former archive and loose all data.

6. Click the *Archive* button ⓓ to back up the project or the *OK* button ⓔ , if you do not need to back up any more files.

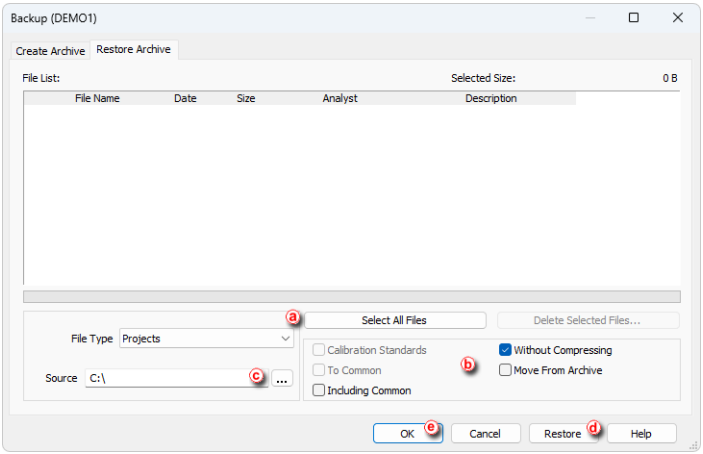
Note: Clicking *OK* will archive current selection.



17.2 Restoring a project from an archive

1. Open the *Backup* dialog by selecting *Instrument - Restore...* in the *Instrument* window.
2. Choose the source directory and select the source file ⓒ . Compressed files will have the .DGZ extension.
3. Select *Projects* in the File Type ⓐ option to restore a complete project directory.
4. Choose from the following options ⓑ :
   - Uncheck the *Without Compressing* option to restore all files from a compressed format.
   - Check the *Move from Archive* option to have the archived files erased after restoring them.
   - Check the *Including Common* option to also restore the COMMON subdirectory.
5. Select the project or projects you wish to restore from the list. The *Select All Files* button ⓐ will select all projects.
6. Click the *Restore button* ⓓ to restore the project or the ***OK*** button ⓔ if you do not need to restore any more files.

Note: Clicking *OK* will restore current selection.

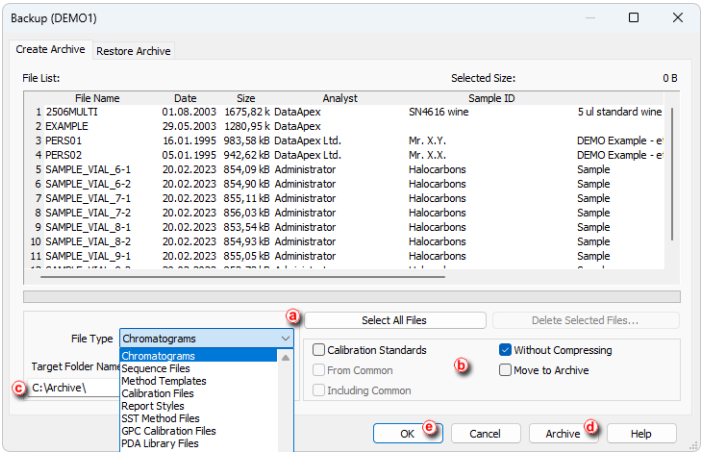


17.3 Archiving specific files (Creating an Archive)

It is strongly recommended to archive the whole project folder after being shelved but it is also possible to archive specific files only. An archive can be made by simply copying the files or by compressing them into one file (*.DGZ format).

1. Open the *Backup* dialog by choosing *Instrument - Archive...* in the *Instrument* window.
2. Select the *File Type* ⓐ option according to the files you wish to archive.
3. Select the files you wish to back up from the list. The *Select All Files* button ⓐ will select them all.
4. Choose from the following options ⓑ :
   - Uncheck the *Without Compressing* option to archive all files into one compressed file.
   - Check the *Move to Archive* option to have the original files erased after backing them up.
   - Check the *Calibration Standards* option when archiving chromatograms. The chromatogram files from the CALIB subdirectory (instead of the DATA subdirectory) should be listed.
   - Check the *From Common* option to display the system files from the COMMON directory.
5. Choose the output directory and name for the archive ⓒ . Compressed files will have the .DGZ extension.
6. Click the *Archive* button ⓓ to back up the file or the *OK* button ⓔ if you do not need to back up any more files.

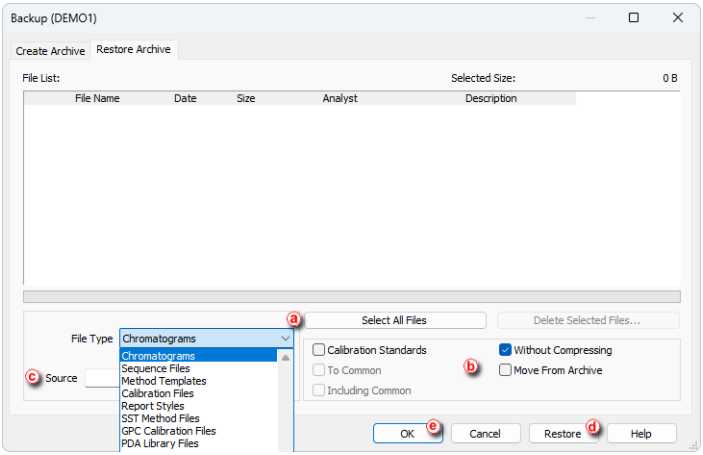
Note: Clicking *OK* will archive current selection.



17.4 Restoring a file from an archive

1. Open the *Backup* dialog by choosing *Instrument - Restore...* on the *Instrument* window.
2. Choose the source directory and select the source file ⓒ .
3. Select the *File Type* ⓐ option according to the files you wish to restore.
4. Choose from the following options ⓑ **:**
   - Uncheck the *Without Compressing* option to restore files from a compressed format.
   - Check the *Move from Archive* option to have the archive files erased after restoring them.
   - Check the *Calibration Standards* option when restoring chromatograms to the CALIB subdirectory (instead of the DATA subdirectory).
5. Select the files you wish to restore from the list. The *Select All Files* button ⓐ will select them all.
6. Click the *Restore* button ⓓ to restore the files or the *OK* button ⓔ if you do not need to restore any more files.

Note: Clicking *OK* will restore current selection.


Backup (DEMO1)
Create Archive
Restore Archive
File List:
Selected Size:
0 B
File Name
Date
Size
Analyst
Description
a
Select All Files
Delete Selected Files...
File Type
Chromatograms
Chromatograms
Sequence Files
Method Templates
Calibration Files
Report Styles
SST Method Files
GPC Calibration Files
PDA Library Files
c
Source
Calibration Standards
To Common
Including Common
b
Without Compressing
Move From Archive
OK
e
Cancel
Restore
d
Help

18 Managing the Chromatography Station

Following chapters contains extended information how to set restrict access to various parts of Clarity to certain users or set up communication with a mobile application.

18.1 Enabling instruments to be used by Clarity2Go application

Clarity enables to send specific parameters over the internet to be monitored via **Clarity2Go** application. In this way you can monitor your analyses while outside the laboratory. Note that both PC with Clarity and smartphone must be connected to internet. For more information regarding Clarity2Go installation refer to www.dataapex.com/product/clarity2go.

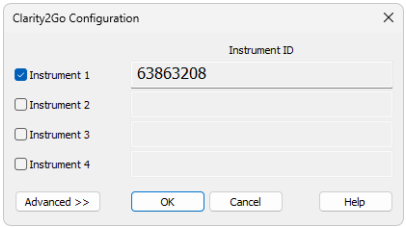
The whole solution consists of three independent parts:

- **Clarity** station (at your side) - sends information about state and running analyses to the server.
- **Server** (at **DataApex's** side) - dispatches the information from **Clarity** stations to **Clarity2Go** clients.
- **Client** (at your side) - device (smartphone or tablet) with installed **Clarity2Go** application processes information from the server.

DataApex is providing a free public server for this use.

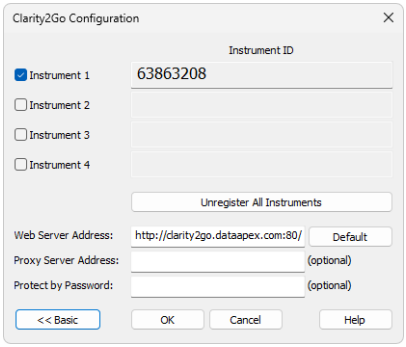
How to set up Clarity:

1. In the *Clarity* main window, go to *System* menu and click on the command *Clarity2Go...*.
2. In the opened *Clarity2Go Configuration* dialog, check the checkbox of *Instrument* 1 to 4, depending on the instruments you want to monitor. Every checked Instrument will get its unique *Instrument ID*.
3. Click the *OK* button to save the configuration and continue with steps described in **How to set up Clarity2Go** section or refer to *Advanced* options bellow.



Options described below are optional and are not obligatory for correct functionality. They are revealed by clicking the *Advanced* button.

- *Unregister All Instruments* - disables the monitoring in the **Clarity2Go** application. Instruments that have been registered will no longer be available for monitoring. If you will later change your mind, you will have to generate new *Instrument ID*.
- *Web Server Address* - do **not** change this field. It defines the address of **Clarity2Go** web server. Address other than default will result in the monitoring to be not functional! Press the *Default* button to set functional web address of the server.
- *Proxy Server Address* - consult with your local administrator if a proxy server is applied in your local network and then provide the proxy server address.
- *Protect by Password* - provided password will be valid for **all** Instruments. The same password needs to be provided in the **Clarity2Go** application to unlock the monitoring.
- Click the *OK* button to save the configuration and continue with steps described in **How to set up Clarity2Go**.



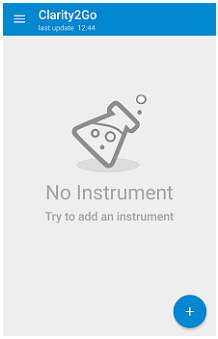
How to set up Clarity2Go:

Once you have configured instrument(s) in **Clarity**, it's time to monitor those instruments using **Clarity2Go** application. This part assumes that you have **Clarity2Go** for Android application installed and running.

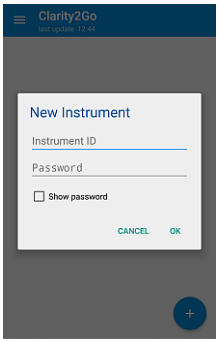
1. Make sure that you are not in the **Clarity Demo** mode, indicated by a gray stripe at the bottom of the application with the inscription **DEMO mode**. Tap on the *TURN OFF DEMO*.

   Note: **Clarity Demo** mode does not allow to add instruments.

2. In the *Settings*, tap on *Demo - Switch to demo mode* which turns the **Clarity Demo** mode *OFF*.
3. Return back. In case you are configuring **Clarity2Go** for the first time, you will see that there is no instrument.



4. Tap on the blue "plus" button at the bottom right corner to add a new instrument.
5. Enter *Instrument ID* that has been generated by **Clarity** and enter password (only if you have set it up in **Clarity**). Tap on the *OK* button to start monitoring this instrument.



6. The newly configured instrument will be added to the list of instruments that are being monitored.

Note: You can invoke the application menu by tapping on the 3 horizontal lines - the menu contains *Settings*, built-in *Help* and *About* options.

18.2 Locking/Auto Locking a Clarity Instrument

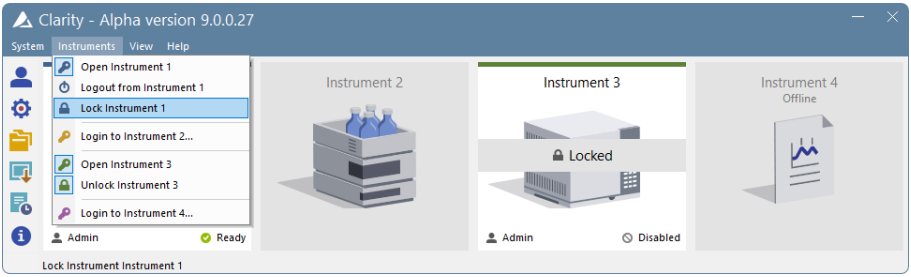
You may lock a Clarity Instrument protected by password if you want to prevent unauthorized access to it, for example, when an analysis is running.

Manual Lock

- Instrument can be manually locked either from *Instrument* window by clicking *Instrument - Lock Instrument_Name*.

  or

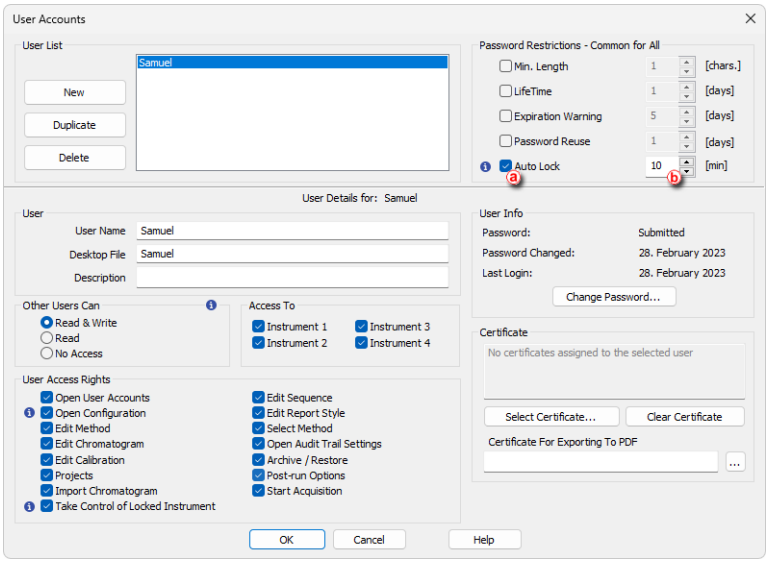
- From the *Main Station* window by clicking *Instruments - Lock Instrument_Name*.



Auto Lock

It is possible to set the automatic lock function so that all opened instruments will be locked after a period of inactivity.

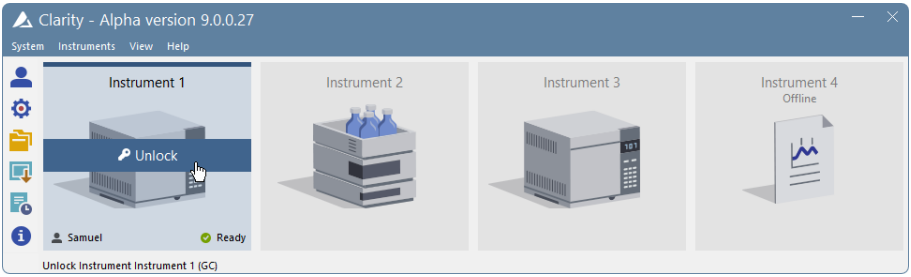
1. Open the *User Accounts* window by clicking on or choose *System - User Accounts*.
2. Check the *Auto Lock* function ⓐ .
3. Set the period of inactivity in minutes after which all opened *Instruments* will be locked ⓑ .



Caution: When an Instrument is Auto Locked, all unsaved changes in modal dialogs (Method Setup, Single Analysis, Report Setup, etc) are discarded and those dialogs are closed.

18.3 Unlocking a Clarity Instrument

1. Select *Instruments - Unlock Instrument 1* from the *Main Clarity* window or click on the *Instrument* image.
2. Enter the password and click OK.

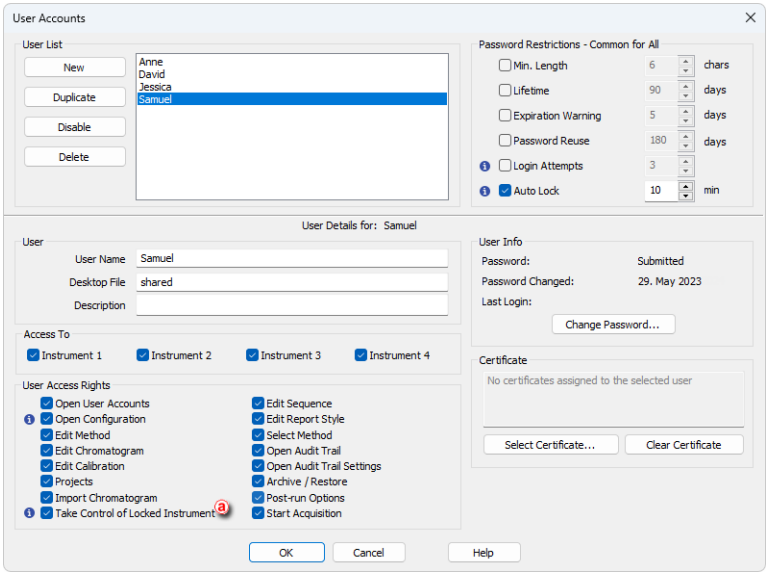


18.4 Taking control of Clarity Instrument

You may take control of an Instrument where a different user is already logged in. To be able to achieve this, the option *Take Control of Locked Instrument* has to be enabled in the *User Accounts* settings for the user who wants to take over.

Setting up the User Right

1. Open the *User Accounts* window by clicking on or choosing *System - User Accounts*.
2. Check the *Take Control of Locked Instrument* in the *User Access Rights* ⓐ part of the dialog for users who should be able to do so.

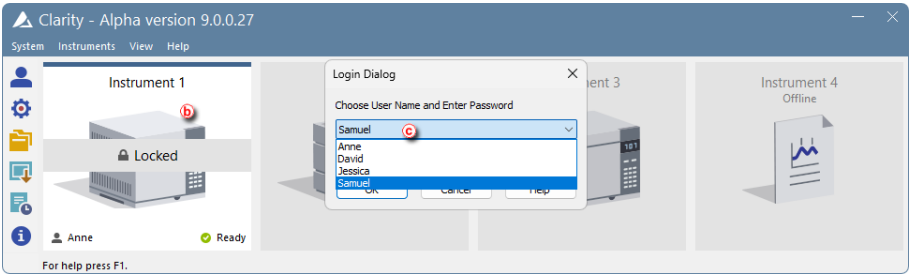


Note: It is recommended to set one common *Desktop File* for all users with this option enabled. Otherwise the desktop of the first logged user will be used for all users that take control over the Instrument, until the Instrument is closed again. It is also recommended to set the same *Edit...* rights for users that plan to take over Instruments (other rights might differ between the users).

Taking Control of Locked Instrument

The steps are similar to the standard logging to instrument.

1. Select *Instruments - Unlock Instrument 1* from the *Main Clarity* window or click on the *Instrument* image ⓑ .
2. Choose your User Name ⓒ .
3. Enter the password and click OK.



Caution: All unsaved changes in files made by the previous user will be discarded.

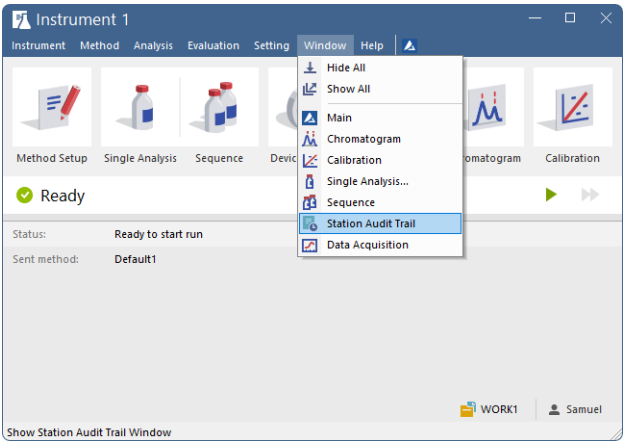
Note: It is possible to take control of a locked Instrument using the Command line parameters. The user *(user=…)* and password *(p=…)* parameters must be included for each command. Althought commands can be run on the locked Instrument this way, the Instrument remains locked.

18.5 Monitoring Events and Operations in Clarity

The ***Audit Trail*** can be used for finding out who did what and when, including file operations, changes to settings, events that take place during data acquisition and system messages. Therefore this is an essential tool for troubleshooting and managing Clarity.

To access the ***Station Audit Trail***:

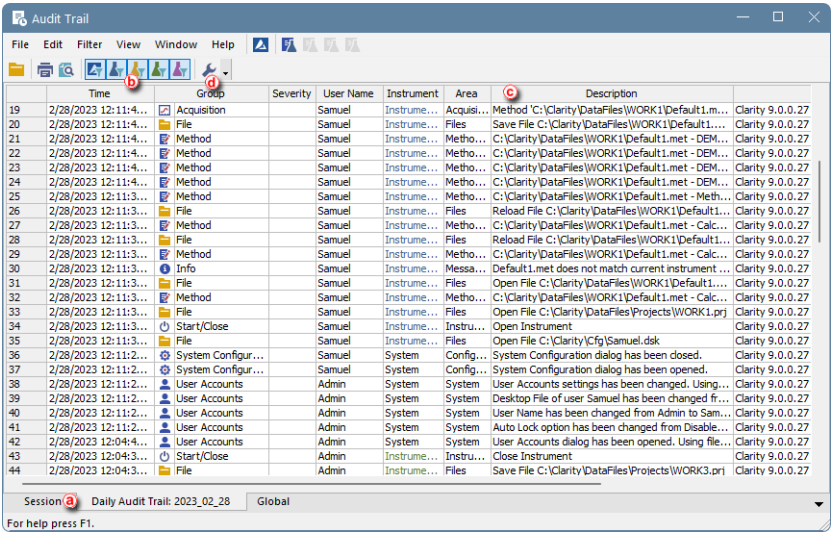
1. Select *Window - Station Audit Trail* from the *Instrument, Chromatogram, Calibration, Sequence* or *Data Acquisition* windows. Alternatively click icon in the *Main Station* window.



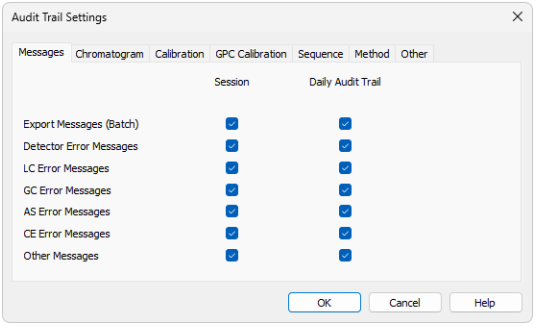
2. Click on the *Session* tab ⓐ if you would like to see the log from the time Clarity was started or on the *Daily Audit Trial* tab for the present day events.

   Note: The *Daily Station Audit Trail* is stored in one separate file every day the station is running. These files can be opened by using the command *File - Open Audit Trail (Append)*.

3. Click on the *Instruments* or *System* icons ⓑ to filter out events and operations based on instrument where they occurred.
4. Inspect the *Description* column to find out about operations and events that have taken place ⓒ .



5. Click on the *Properties* icon ⓓ to set up which events and operations should be recorded in the *Session* or *Daily Audit Trail*.



To access the file-specific *Local Audit Trail* (Chromatogram, Calibration, Sequence and Method):

1. Select *Window - Chromatogram, Calibration or Sequence Audit Trail* from the corresponding window or click on the *Audit Trail* icon in the *Method Setup* window to open corresponding *Audit Trail*.

Note: The *Local Audit Trails* are included in the *Chromatogram, Calibration, Sequence* and *Method* files and contain the whole file history.

18.6 Controlling Clarity from an external application

It is possible to send commands to **Clarity** using Windows command line parameters and also to read its status through Windows Dynamic Data Exchange (DDE).

- For more information on the commands go to our List of commands in the **Clarity Reference Guide**.
- You can also find the list of variables which will give you information on Clarity status on our DDE datasheet.

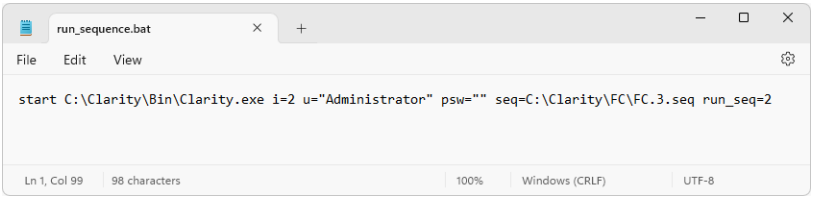
18.7 Starting a sequence from Clarity at a defined time

It is possible to schedule a task that will run **Clarity** with defined parameters to start a sequence measurement automatically. To achieve this, proceed as follows:

1. Prepare a batch script file (e.g., RUN-SEQUENCE.BAT) to perform the required tasks via command line parameters

   The batch file should contain the following line (example):

   start C:\Clarity\Bin\Clarity.exe i=2 u="Administrator" psw="" seq=C:\Clarity\FC\FC.3.seq run_seq=2



   Explanation:

   - *start C:\...\Bin\Clarity.exe* will start Clarity from the specified root directory
   - *i=2* will open the desired instrument (2)
   - *u="Administrator" psw=""* will log in the specified user using the password provided (necessary even if the password is empty)
   - *seq=C:\...\SequenceName.seq* specifies the sequence to be run
   - *run_seq=2* starts the sequence on the desired instrument (2)

2. Prepare the sequence to be run

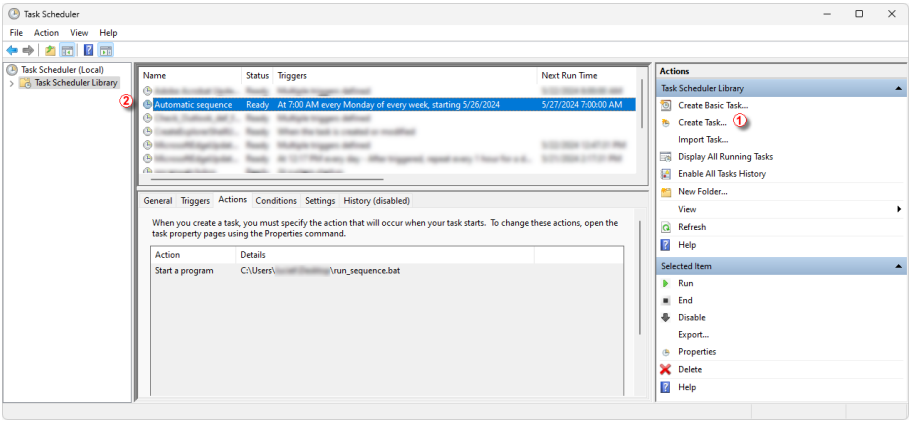
   Set the sequence as necessary for your analysis. The sequence can contain just one row with a start-up method, or additional rows with standards/samples for measurement. The start-up method should prepare the devices for measurements, e.g., switch on the detector lamps, flush the systems as required for equilibration, etc.

3. Use the *Task Scheduler* to schedule starting of the batch script (Windows 11)

   To schedule running the RUN-SEQUENCE.BAT at a specific time and date, use the Windows app *Task Scheduler*. After creating a new task (*Actions* section - *Create Task...* ①), apply the following settings in the *Create Task* dialog:

- tab *General*: set the name of the action (e.g., Automatic sequence), choose the *Run only when user is logged on* option (and do not log yourself off when leaving the PC).
- tab *Triggers* - *New...*: set the date and time of running the script, eventually use further advanced settings to fine-tune the task scheduling (e.g., repeating).
- tab *Actions* - *New...*: choose the *Start a program* option a browse to select the prepared batch script.

The created task is now present in the *Task Scheduler Library* ②. If Windows Updates are available, remember to install them manually (automatic OS updates might log you out due to PC restart - this would prevent the task to be started by the *Task Scheduler*).



19 Clarity in specific scenarios

In this chapter, there are SOPs, that helps you set up Clarity in not-so-usual scenarios, outside of chromatographic laboratory.

19.1 Clarity in the classroom

This section focuses on configuring Clarity to simplify its use in classrooms and students' laboratories, particularly for teaching scientific principles and lab workflows. It explains key settings, like students' account management and evaluating the data on another PC than it was measured on (e.g., in the classroom). In addition there is also tip, how to make your lesson for bigger groups more engaging with some hands-on experience, e.g., to use instrument simulation modes to simulate real measurement.

19.1.1 Creating User Accounts

In *User Accounts* dialog, set up one or more teacher account(s), with complete privileges, and one or more student accounts with limited privileges. Recommended limitation of privileges is access to *User Accounts* and *System Configuration* - so the students can't change privileges of any account, and change configuration of connected devices. Any other limitations depends on what students should perform in your specific use case, e.g., restricting *Edit Method* when student should just use already existing method and not develop new one.

More detailed info on how to set the user accounts can be found in Create New User Account and Restricting Access topics.

19.1.2 Setting the directories

If you want save the files on shared disk to enable access from another computer in the same network, e.g., from the classroom or office. You can set the directories accordingly in the *Instrument Directories for Projects* dialog accessible from main Clarity window.

More detailed info on how to set the directories can be found in Working with Directories topic.

19.1.3 Transferring the projects

It also may be needed to transfer existing project to different disc where you set directories in previous step. To do that, you can simply copy/move whole project (including *.prj file) in File Explorer, or use *Archive/Restore* feature.

More detailed info on how to transfer the project to another disc can be found in *Migrating Projects* topic.

19.1.4 Backing up important files

It is recommended to back up important files, so in the case that any unexpected issue occurs (e.g., someone accidentally power off the computer while Clarity is still

running), and important files are corrupted or deleted, it is simple to get the settings back as it was before.

List of recommended files for back up:

- Clarity.cfg + any other configuration file present in Cfg directory.
- Clarity.dsk + any other desktop file present in Cfg directory.
- Clarity.psw in Cfg directory.
- optional: method(s) validated and used for measurement

19.1.5 Bonus Tip: Simulated Measurement

To showcase Clarity workflow, and simulate laboratory process for larger group of students without need of physical connection to laboratory instruments, you can use Clarity Demo version, accessible from our website www.dataapex.com. In the Demo version, there is simulated connection to any available device you configure on the *Instrument*, so the students can get familiar with Clarity and the work they will do in the laboratories.

20 Utilities

Clarity installation contains various utilities for validating the installation or predefining various Clarity profiles which helps you in using more configurations of laboratory instruments.

20.1 Checking that the software has been installed correctly (Installation Qualification - IQ)

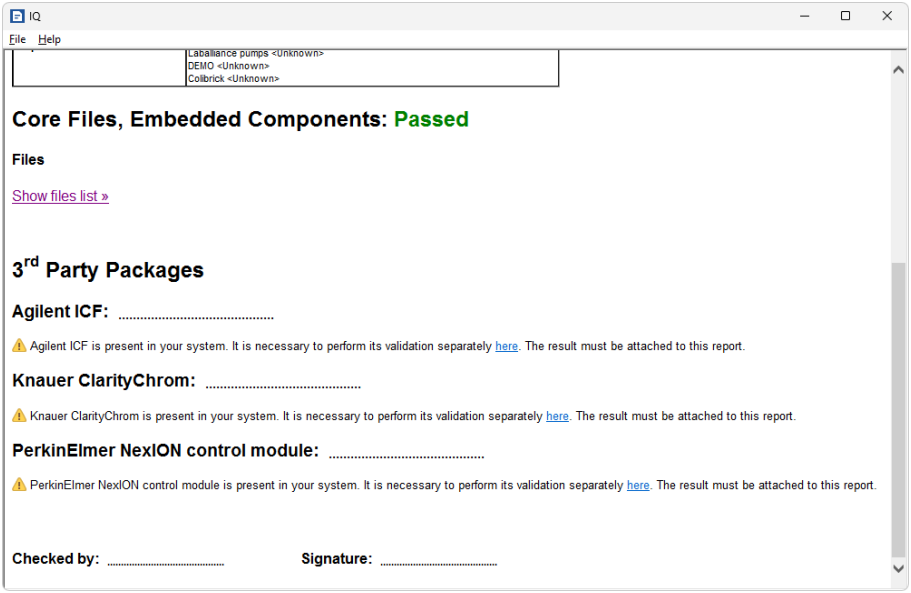
The *Installation Qualification* (**IQ**) is a procedure confirming that the software has been installed successfully and that correct versions of files are present.

1. Install the Clarity station according to the instructions of the *Installation Wizard*.
2. After the installation has been completed, you can open *IQ* by searching for *IQ Report* in the search field of the Start menu. Alternatively you can start *IQ* by using C:\CLARITY\BIN\IQ.EXE.
3. If the installation has been correctly performed, the status should read: "*Installation Qualification Test: Passed*".
4. If the Installation Qualification fails, it is recommended to uninstall and then re-install Clarity. If it fails again, contact DataApex support.

   Note: You can use *Show files list* to display list of all validated files and search for the ones that are causing issues.

5. The *Installation Qualification* report can then be printed, copied to the Windows Clipboard or sent as an email.

Caution: Some driver packages have standalone IQ that must be performed separately by clicking *here* in given section. Clarity IQ is **NOT** valid unless IQ of all components passed and reports are stored together.

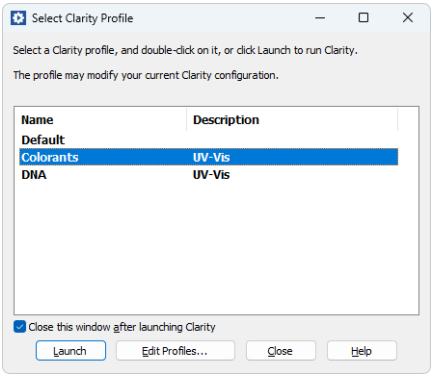


Note: The most common reason for a "Failed" result is the installation of an updated version over an existing installation of Clarity. This itself does not produce any errors but since some of the files are preserved from the original installation, the checksums will not match.

20.2 Editing Clarity profiles for different analyses using the Launch Manager

Launch Manager is a utility that allows you to start the Chromatography Station with specific setting. The collection of these settings is saved as a *Profile* in *Launch Manager*. You can select specific configuration, desktop file containing custom calculations and which instrument and project specifc user will be asked to log in.

1. Start the *Launch Manager* either from the Windows Start menu or using C:\CLARITY\BIN\LAUNCHMANAGER.EXE.
2. Click on the *Edit Profiles* button to create or modify the profiles.



3. Select a profile ⓐ to modify it or click on the *New* button to create a new profile ⓑ .
4. If you created a new profile, fill its name. For easier orientation it is recommended to fill in the *Description* which eases the distinguishing of different profiles.
5. Select the configuration file that will be loaded after the start of Clarity ⓒ .

   Note: The list of configuration files is retrieved from the installation directory (configuration files are located in C:\CLARITY\CFG by default). Clicking on » button opens menu for managing the configuration files, see Creating a duplicate configuration using the Launch Manager for one example of usage.

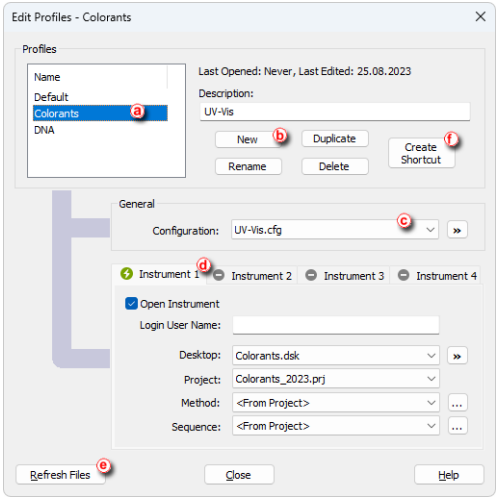
6. If you select the <Last Used> option, Clarity will start with the last configuration it was opened with or if Clarity is running, the present configuration will be preserved.
7. For each Instrument, choose if it should be opened at the Clarity start by *Open Instrument* checkbox. Select the User, Desktop, Project, Method and Sequence files that will be loaded when opening instruments.

   Note: In the desktop file, all layout setting is saved (the width of the table columns, the custom toolbars), but also custom calculations created in *User Columns*.

   Note: If <From Project> is selected, the Method and Sequence that were last opened in selected Project will be used.

8. You can use *Refresh Files* button ⓔ to reload all the files displayed in the *Edit Profiles* dialog.
9. Once the profile is configured, *Close* the *Edit Profiles* dialog and *Launch* the profile either by double clicking on the profile or by selecting a profile and clicking on the *Launch*.

Note: You can use *Create Shortcut* ⓕ to place shortcut on the desktop which can be directly used to launch given profile.

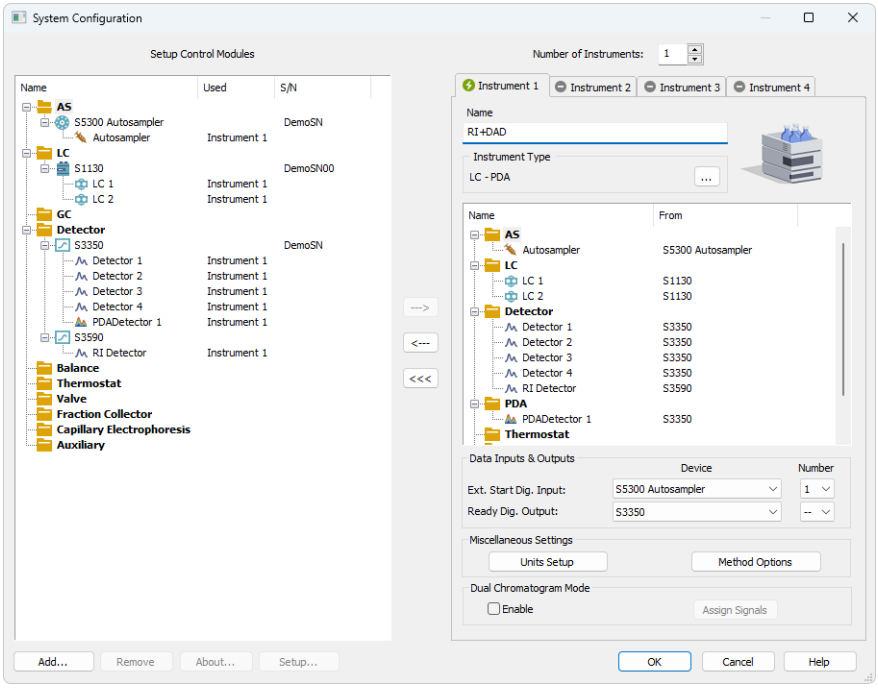


20.3 Creating a duplicate configuration using the Launch Manager

This topic describes how to create a duplicate configuration using the *Launch Manager*. This becomes especially handy when you have system with two detectors (e.g., RI + DAD) but you don't need to run them together every time.

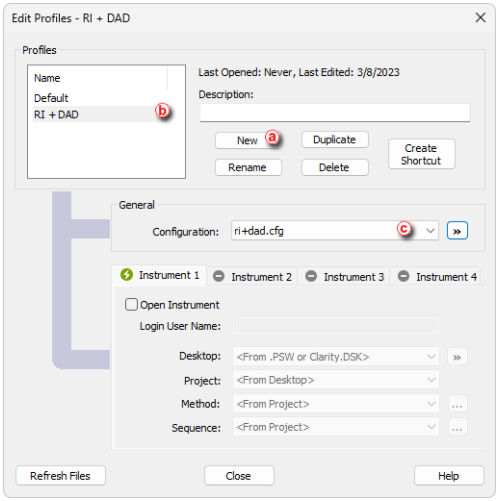
1. If you don't have any configuration yet, start Clarity and configure your device(s) according to the chapter "Adding a new device" and close Clarity. Otherwise start with the next step.

   Note: In this example we start with LC system with both DAD and RI detectors configured.

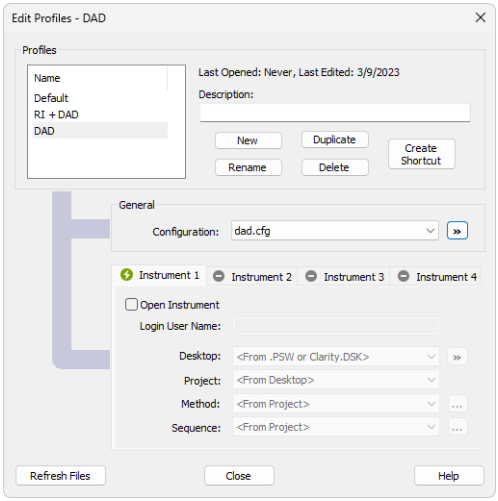


2. Open *Launch Manager* either from the Windows Start menu or by using C:\CLARITY\BIN\LAUNCHMANAGER.EXE.
3. In the *Select Clarity Profile* dialog click *Edit Profiles...*.
4. In the *Edit Profiles* dialog, click the *New* button ⓐ to create a new profile and name your profile (e.g. *RI + DAD*). Click *OK* to save the profile. Newly created profile is displayed in the small table on left ⓑ .
5. From the drop-down list ⓒ , select CLARITY.CFG, click the » button, from the selection choose *Duplicate* and in the following dialog name your configuration (e.g. ri+dad.cfg).

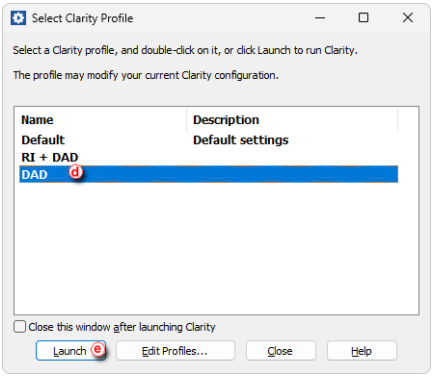
Note: This step will create a duplicate configuration (.cfg file) based on the current Clarity setup (as described in step 1.).



6. Create a new profile (DAD) with a different configuration (duplicated ri+dad.cfg named as dad.cfg), similarly to steps 4.-5. Once done, your profile should look similar to the image below.

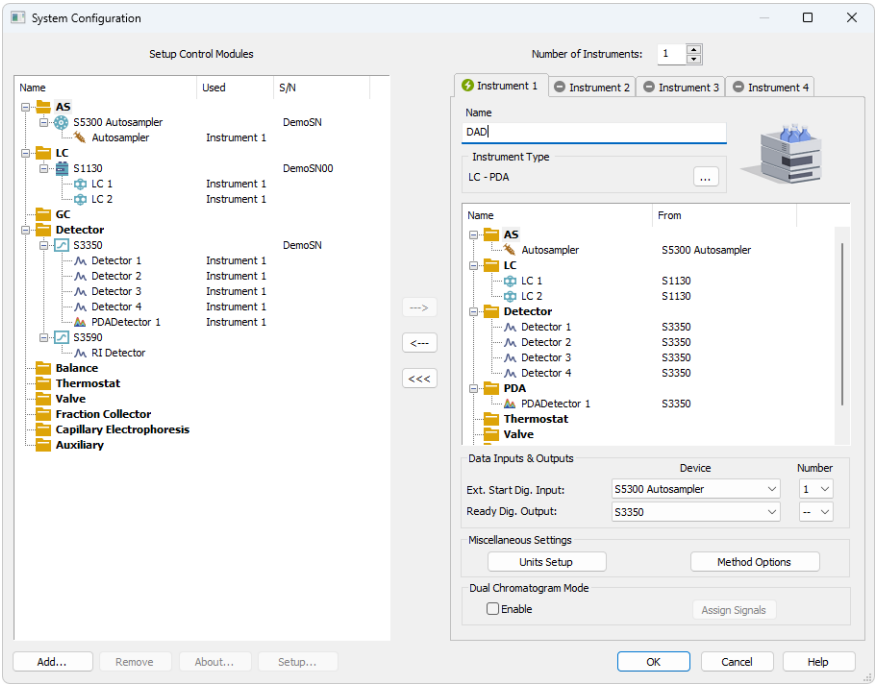


7. Close this dialog to return to the main *Launch Manager* window.
8. In the *Launch Manager* window select the *DAD* profile ⓓ which has not been configured but simply duplicated and click on the *Launch* ⓔ button.



9. Clarity has launched with the selected profile, open *System Configuration*. Since the configuration has been duplicated from the initial configuration, both detectors are present. Remove the RI detector from instrument and save the configuration by click *OK* in the *System Configuration* window.

   Note: This step may differ based on used control modules. In our case simply drag the RI module from right side to the left one. In other modules e.g., when using ICF you have to invoked the control module setup and change it there.



10. Launch each profile using the *Launch Manager* to make sure that correct configuration is loaded.

21 Best Practices for Using Clarity Effectively

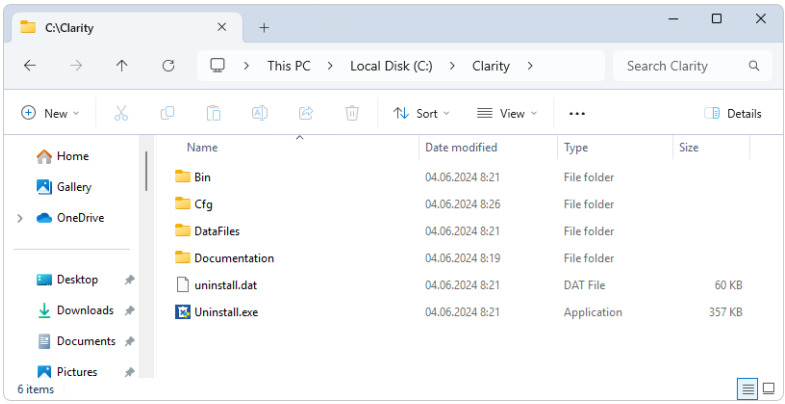
To ensure Clarity operates smoothly and delivers accurate results, it is important to follow certain practices when working with the software and your computer.

These principles cover topics like maintaining Clarity's file structure, proper data management, and adhering to recommended workflows. This section introduces these foundational guidelines, which help avoid errors, prevent data loss, and ensure a seamless experience.

21.1 Respect Clarity's file structure

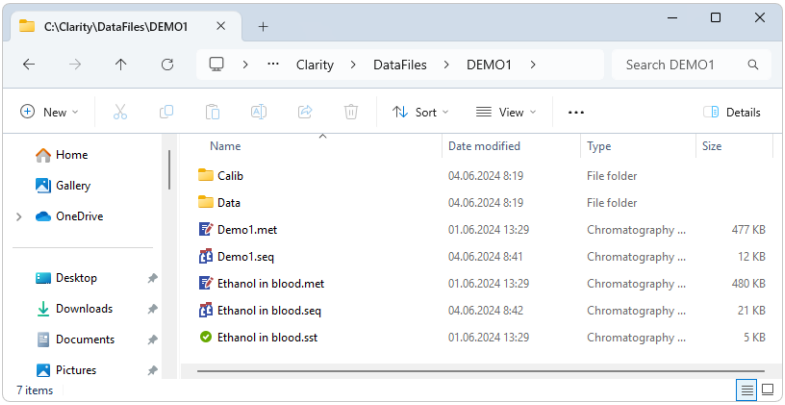
Maintaining Clarity's file structure is crucial for ensuring smooth operation and reliable data acquisition. The Clarity folder includes four subfolders:

- *Bin Folder* contains executable files for the software and tools like Launch Manager.
- *Cfg Folder* stores software configurations, audit trails, and diagnostic data. Important files like .cfg, .dsk, and Clarity.psw should be backed up regularly.
- *Data Files Folder* organizes chromatographic data using a project- based structure. Each project has its own folder with subfolders for calibrations and sample data.
- *Documentation Folder* provides datasheets and manuals specific to your version.



The Data Files folder stores chromatographic data using a project-based approach:

- *Projects Folder* contains **.prj* file for each project.
- *Common Folder* stores shared files, such as report styles **.sty*, and templates, accessible to all projects.
- *Individual Project Folders* contains all the files belonging to each project in this structure:
    - *Calib Folder* holds calibration **.cal* files and standard or blank chromatograms.
    - *Data Folder* contains chromatograms of unknown samples.
    - The root project directory contains method **.met*, sequence **.seq*, and SST **.sst* files.



Subfolders can be created in Data and Calib folders for organization of chromatograms, for more details see Storing chromatograms into subfolders topic. However, avoid adding folders directly to the project folder or storing files outside of this structure, as this may disrupt file linking and cause errors, if you want to change the location of Data Files directory it can be done in the Directories dialog, for more details see Setting up project directories topic.

21.2 Avoid switching Windows OS users and entering Sleep mode

Switching Windows user profiles or entering sleep mode while Clarity is running can disrupt communication with the hardware key or connected instruments. Active Clarity station (with an Instrument window open) prevents entering the sleep mode to ensure reliable data acquisition. However, in some BIOS configurations, this safeguard may fail.

To avoid issues, do not switch users while Clarity is active, and disable Power Saving features in both Windows OS (for all users) and the BIOS settings.

21.3 Protect Clarity from unexpected shutdowns

Unexpected computer shutdowns, such as those caused by Windows updates, power outages, or forced restarts, can interrupt ongoing measurements and potentially corrupt critical files that store station settings.

To minimize the risk of loss of settings or its corruption:

- Regularly back up important files stated below.
- Schedule Windows updates during off-hours when Clarity is not running to prevent forced restart.
- Ensure reliable power through a UPS (Uninterruptible Power Supply).

List of recommended files for back up:

- Clarity.cfg + any other configuration file present in Cfg directory.
- Clarity.dsk + any other desktop file present in Cfg directory.
- Clarity.psw in Cfg directory.
- optional: method(s) validated and used for measurement

22 Troubleshooting

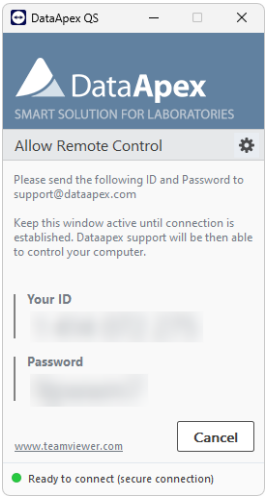
This chapter contains a set of Standard Operating Procedures (SOPs) designed to assist you in resolving any issues you may encounter while working with Clarity. The SOPs include instructions on which information and data to collect and sent to our Support team, enabling them to offer effective solutions to your problems.

Note: Video tutorials and How To videos regarding Troubleshooting can be found in the Troubleshooting playlist on our YouTube channel.

If you do not find your answers here, use the www.dataapex.com website where the *Support* menu will navigate you to video tutorials, frequently asked questions (FAQ), and the *Support request form*. Alternatively, you can contact your distributor or the **DataApex** helpdesk via e-mail. Please note that we can request the collection of some configuration files. In case you have an e-mail client installed, you can collect these files using the *Help - Send Report by E-mail* menu in the main **Clarity** window.

Solutions to problems connected to particular **hardware** can be found in the corresponding manuals.

As the last option when troubleshooting complicated issues, **DataApex** may provide remote support via **TeamViewer QuickSupport** to registered customers (paid sevice). To use this option, the user must first contact **DataApex Technical Support** (support@dataapex.com). The **TeamViewer QuickSupport** application can be downloaded by clicking *Help - TeamViewer QS* in the main *Clarity* window. The application is ready to be used directly after downloading.



22.1 Missing HW key

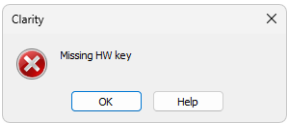


Fig. 1: Missing HW key error dialog

If you try to start **Clarity** without the key, an error message saying "Missing HW key" is displayed and **Clarity** will not start. The key must be plugged into a USB port and its driver must be properly installed. Under normal circumstances, USB drivers are automatically installed upon inserting the key into a USB port.

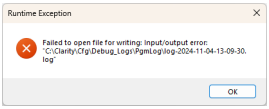
Reason 1: Your HW key may not be connected correctly.

Solution: Check if the key is properly inserted in the USB port. Check whether the USB port is working (e.g., try to connect a different device, etc.), check if the HW key diode is lighting steadily, if blinking or is dimmed try another USB port.

Reason 2: Your HW key may not be installed properly.

Solution: In the *Windows Control Panel - System and Security*, select the *System* icon, access the *Device Manager* tab, and look for the **Universal Serial Bus Controllers** - **Rockey4** item. In some cases, it can be found also directly in the root folder of the device manager. If it is not there, unplug and plug in the HW key again to the USB port.

22.2 Failed to open file for writing



For Clarity to operate correctly, the logged-in Windows User must have *Read* and *Write* access privileges to the entire Clarity folder. Without these permissions, Clarity cannot be started.

Reason: You probably have insufficient access rights to the C:\CLARITY directory.

Note that this solution requires a user with administrator rights.

- Right-click on the C:\CLARITY directory and choose *Properties*.
- In the *Clarity Properties* on the *Security* tab, locate the User/Group of Users and click *Edit*.
- Provide the administrator password when prompted.
- In the next dialog, grant the User/Group of User the necessary permissions by checking the *Allow* option for: *Read & Write*, *List folder contents*, and *Read*.

In case insufficient privileges are applied only to a part of the Clarity folder, Clarity still may not work properly, causing similar error messages to pop up.

22.3 The User Code is not accepted

The User Code is not accepted and thus Clarity cannot be started. In the case the User Code is intended for unlocking additional extensions/add-ons for the station, the previously used accepted one is still saved.

If necessary, contact the manufacturer or your distributor to request the correct User Code. In this case, be prepared to provide the serial number (S/N) of the workstation.

Note: The *User Code* dialog does not distinguish between upper case and lower case letters. However, be careful not to confuse the letter "l" with the number "1".

22.3.1 The User Code is not valid for version x.y

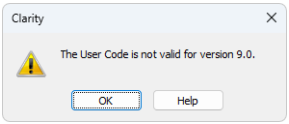


Fig. 2: The User Code not valid for version error dialog

Reason: You have probably entered a User Code for a different version.

Solution: You have to enter the User Code corresponding to your current version. For example, when you purchase additional extensions/control licenses, a new User Code is generated for your station. The new User Code is valid only for the most recent Clarity major version, so you will probably need to install the latest version of the software.

22.3.2 Wrong User Code

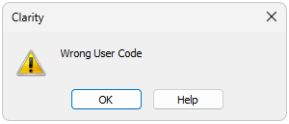


Fig. 3: Wrong User Code error dialog

The User Code of the workstation does not match the code in the HW key.

Reason: You have entered a User Code that does not match the serial number of the HW key plugged into the PC.

Solution: Submit a correct User Code. The User Code can be found on the back of the plastic card provided with the installation USB.

22.3.3 Wrong Software Version

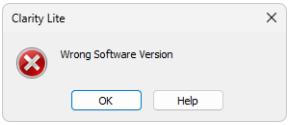


Fig. 4: Wrong Software Version error dialog

Reason: You have probably installed a different application than you had purchased. For example, you installed Clarity Lite instead of Clarity.

Solution: Install the correct application you had purchased. If you are not able to locate the correct installer, contact the manufacturer or your distributor.

22.4 Trial Expired

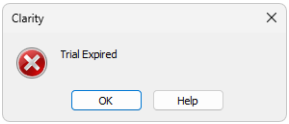


Fig. 5: Trial Expired error dialog

The Trial period (time period when Clarity works without a User Code filled in) expired. You are prompted to enter a User Code or a Trial Prolongation Code.

Reason: Your Clarity station just ended its trial period.

Solution: a) Enter the correct User Code, which switches Clarity from the Trial mode into the full mode ①

b) Or switch to section ② and enter a Trial Prolongation Code to extend the trial mode period. Trial Prolongation Codes must be requested from your distributor or DataApex.

Once a correct User Code or Trial Prolongation Code has been provided, click the *OK* button to start Clarity.

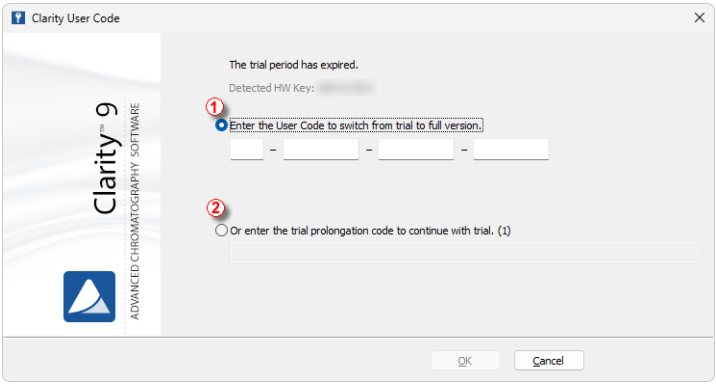


Fig. 6: Clarity User Code

In the case you need to enable trial on the station where the User Code was previously entered check the *D037 Clarity Trial-Full mode switching* datasheet.

22.5 The XX file is corrupted or missing

In most cases, corruption happens when Clarity is unexpectedly closed, e.g., due to power outage or Windows updates forcing the system to restart, or when some important file is moved outside of the expected location. The type of the file indicates the severity of the situation. In majority of cases, Clarity is restarted and a backup file is used instead.

To prevent the problems caused by the corrupted files, we recommend following of the tips in the Best Practices for using Clarity effectively chapter, especially backing up of important files regularly.

22.5.1 Clarity.psw file

The Clarity. psw file holds the information about user accounts. If it is corrupted, Clarity cannot be started.

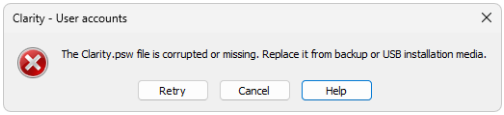


Fig. 7: The Clarity.psw file is corrupted or missing.

- In the case you have backed up the file previously, replace the corrupted .psw file in the *Cfg* folder of your Clarity station, and the *User Accounts* saved in the backup will be ready to use.
- If you have not backed up the .psw file, you have to use the default backup from the CFG\BACK folder or from the USB installation media. In this case, you will have to set up the *User Accounts* again.

22.5.2 Configuration *.cfg file

The configuration *.cfg files holds the information about the setting of the directories, the devices configured on Instruments, and some additional settings that is done in the *System Configuration* dialog.

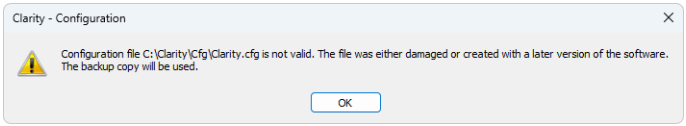


Fig. 8: Configuration file x.cfg is not valid. The file was either damaged or created with a later version of the software.

To repair the damage, follow this process:

1. Open the *System Configuration* dialog and configure your system manually (eg. add detectors, LCs, GCs, valves and so on to the configuration), fill in their settings and distribute them to particular instruments.
2. Close the *System Configuration* dialog by clicking OK.
3. If you had the *Directories* dialog set before, set it once more. Then, close the dialog.
4. Open the Instrument and select the Project that was used before.
5. Check the used methods. If you did not saved the methods in the time the loaded backup configuration was empty, they should have the correct settings as before the problem.

22.5.3 Project *.prj file

The project file contains only information about the last opened documents that are "prepared" for you when you log in next time, so no damage to your data has been done upon corruption. The easiest way to fix this is to delete the corrupted project file and create a new one with the same name.

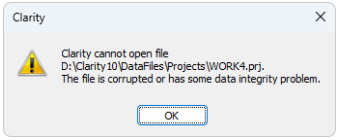


Fig. 9: Clarity cannot open file x.prj.

1. Close Clarity.
2. Find the corrupted file using the File Explorer and delete it - by default it is located in the DATAFILES\PROJECTS subfolder.
3. Go back to Clarity.
4. When logging in to an *Instrument*, select *New Project*.
5. Fill in the same name as the corrupted project had.
6. Confirm that the directories exist and you want to create the project file.

22.6 Data Acquisition - Disabled

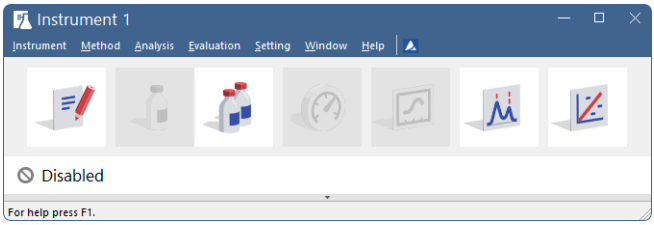


Fig. 10: Data Acquisition disabled

The "**Disabled**" label appears, and the *Single Analysis* dialog and *Data Acquisition* windows are not available. Other manifestations of this error are also: ***Method Setup - Acquisition*** tab missing, *Run*, *Stop*, and *Abort* commands non-functional in the ***Sequence*** window.

Reason 1: No detector is allocated to the Clarity Instrument.

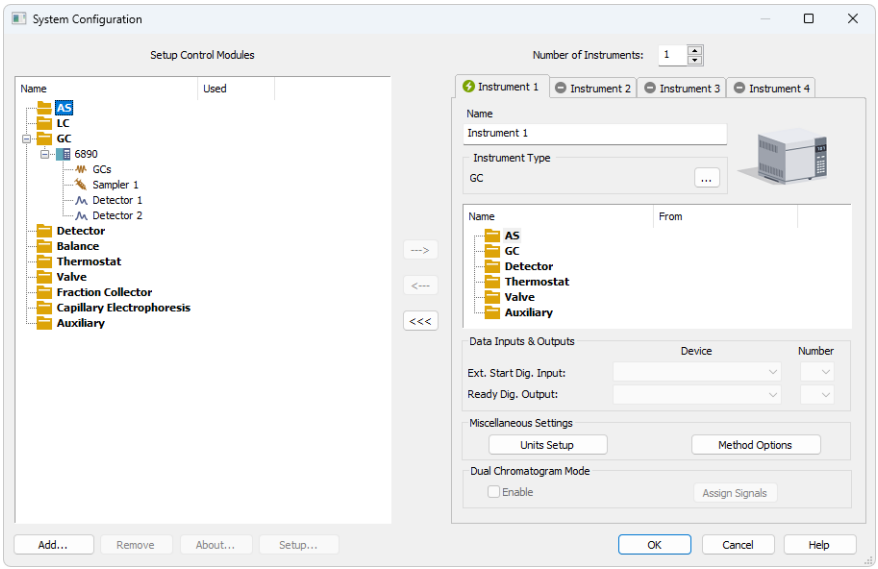


Fig. 11: Detector not allocated to the Instrument

Solution: Open the ***System Configuration*** dialog from the ***Clarity*** window using the *System - Configuration...* command and check the tab of the corresponding Instrument - **Instrument X**. If it has no allocated detectors, add them.

In the list on the left side of *Setup Control Modules*, select the correct detector, and drag it to the corresponding instrument section on the right.

If the appropriate detector is not in the list, add it using the *Add* button and repeat the previous step.

Reason 2: You purchased a license for data collection on fewer Instruments.

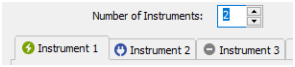


Fig. 12: Small number of Instruments purchased

Solution: Open the *System Configuration* dialog from the *Clarity* window using the *System - Configuration...* command and check the tab of the corresponding Instrument - **Instrument X**. The icon indicates that the Instrument is not available for data acquisition. If you want to use this Instrument for data acquisition, contact your distributor and order an Add-On Instrument.

Reason 3: You are using the Clarity Offline version, which is not intended for data acquisition.

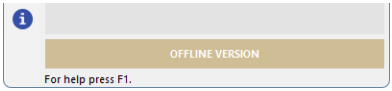


Fig. 13: Clarity Offline

Solution: Check whether there is a brown band with the text **OFFLINE VERSION** on the main *Clarity* window under the instrument icons. If it is, remove the HW key with the **Offline** license and insert a key with the **Clarity** full license.

22.7 Data Acquisition - Simulated

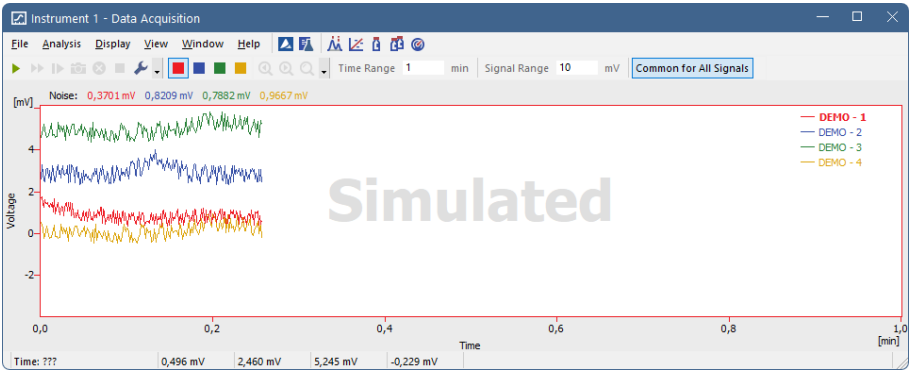


Fig. 14: Data Acquisition Simulated

The title "**Simulated**" is displayed. The corresponding Instrument only displays a simulated curve in the *Data Acquisition* window.

Reason 1: You are using Clarity Demo version.

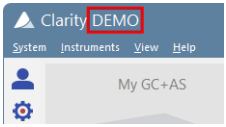


Fig. 15: Clarity DEMO

Solution: Check whether the title **DEMO**is in Clarity window header. If so, uninstall the demo version and install the full version of Clarity.

Reason 2: A DEMO detector is allocated to the Instrument.

Solution: Open the *System Configuration* dialog from the *Clarity* window using the *System - Configuration...* command and check the tab of the corresponding Instrument - **Instrument X**. If it obtains detector signals only from the **DataApex DEMO** detector, it is necessary to reconfigure it. You can find more information on how to add a detector in the chapter "Configuration"

22.8 Clarity is unable to find HW key

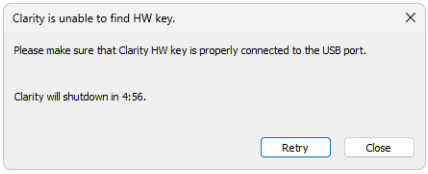


Fig. 16: Clarity is unable to find HW key

When **Clarity** has lost communication with the HW key, the "Clarity is unable to find HW key" error message is displayed. The user has 5 minutes to try to reestablish the communication between Clarity and the key. Once this time elapses, Clarity will automatically shut down.

Retry
Check for the HW key again and resume running **Clarity** in case it was detected.

Close
Close **Clarity** Chromatography Station.

There are two possible explanations for this error message:

Reason 1: The key was removed while *Clarity* was running.

Solution: Plug the key in again. Click the *Retry* button to reestablish the communication.

Reason 2: The USB port which the key is plugged in entered the sleep mode.

Solution: Go to *Start - Control Panel - Hardware and Sound - Device Manager* , locate **Universal Serial Bus Controller**. Right-click each **USB Root Hub** item and choose *Properties*. Click the *Power Management* tab and uncheck the box for "Allow the computer to turn off this device to save power".

Caution: Another way to forbid USB ports from entering the sleep mode is in **BIOS**. This option is however recommended only for **advanced** users and is usually performed by the local System Administrator.

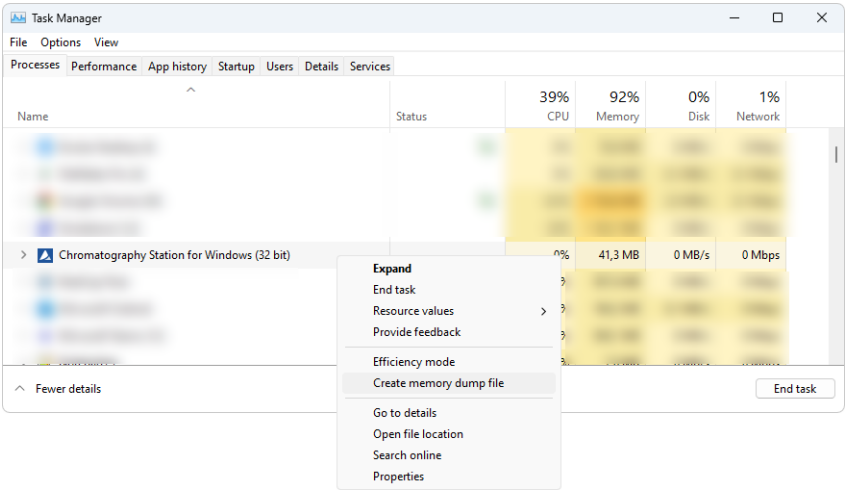
22.9 How to create a dump (*.dmp) file from running Clarity

Sometimes if you encounter problems while working with Clarity, you may be asked by our Support team to provide a dump (*.dmp) file created from the problematic

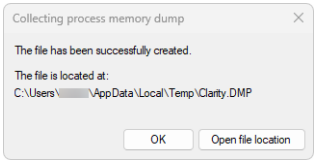
Clarity process. Specifically, this is useful when you are encountering freezes during Clarity operations.

Here is a simple guide on how to create such dump file:

1. Run the 32-bit Task manager with the option Run as administrator (Clarity is a 32-bit process thus the 32-bit Task Manager must be used), it is located here: C:\WINDOWS\SYSWOW64\TASKMGR.EXE.



2. Locate the Clarity process, right click on it, and in context menu select *Create memory dump file*.
3. Wait a moment.



4. A dialog informing that the dump has being successfully created will pop up, including information on where it is located.
5. Send this file to our support team either via email support@dataapex.com, or the Support Request form on our website.